



Professor Steven G. Louie
Professor of Physics, University of California at Berkeley
Senior Faculty Scientist, Lawrence Berkeley National Lab
USA



Lawrence Berkeley National Laboratory



UNIVERSITY OF CALIFORNIA

JEFFREY B. NEATON
DIRECTOR, MOLECULAR FOUNDRY
Lawrence Berkeley National Laboratory
1 Cyclotron Road, 67-3115
Berkeley, CA 94720
jbneaton@lbl.gov
<http://foundry.lbl.gov>

PROFESSOR OF PHYSICS
University of California, Berkeley
543 Birge Hall
Berkeley, CA 94720
jbneaton@berkeley.edu
+1 510-486-4527

December 16, 2017
World Cultural Council -- 2018 Albert Einstein World Award of Science

Dear Members of the Selection Committee,

It is my great privilege to hereby nominate Professor Steven G. Louie of the University of California, Berkeley, for the 2018 Albert Einstein World Award of Science for his seminal contributions to the quantum theory of excited-state properties and to groundbreaking discoveries of novel materials and nanoscale phenomena.

Professor Steven G. Louie is one of the most original and influential theorists in condensed matter and materials physics worldwide. He is a trailblazing leader who has advanced the frontiers of several fields by developing new concepts, pioneering critical theoretical and computational methods that are now in widespread use, predicting new properties and materials, providing insights into novel phenomena, and fostering interactions between theory and experiment. In particular, his breakthrough work on the *ab initio* GW approach single-handedly ushered in the era of first-principles study of excited-state properties of real materials, an indispensable and long-awaited development for computational materials research.

He has trained generations of outstanding students and postdocs, many of whom are now leading research groups at the very best institutions worldwide. An Albert Einstein World Award of Science would recognize his many seminal and far-reaching contributions that have expanded the basic knowledge and shaped the scope of condensed matter physics, materials science, and nanoscience over the past three decades. His achievements will remain a landmark for many scientific generations to come.

As supplements to this nomination letter, please find enclosed two reference letters and a 2-page statement of Professor Louie's scientific achievements, giving a more detailed description of his many groundbreaking contributions. Enclosed also are Professor Louie's CV, a list of his 10 most important papers, a list of all publications, and his recent photograph.

Thank you for your consideration of this nomination, and please do not hesitate to contact me at any point during the selection process. I look forward to hearing from you.

Sincerely,

Jeffrey B. Neaton
Associate Laboratory for Energy Sciences, Lawrence Berkeley National Laboratory
Director, Molecular Foundry, Lawrence Berkeley National Laboratory
Professor of Physics, University of California, Berkeley



Dec. 1, 2017

Selection Committee
"Albert Einstein" World Award of Science
World Cultural Council

Re: Nomination of Prof. Steven Louie for the World Award of Science

Dear Colleagues,

I am writing to express my strongest support for the nomination of Professor Steven Louie of the University of California and Lawrence Berkeley National Laboratory for the "Albert Einstein" World Award of Science. Prof. Louie has had a revolutionary impact on our ability to understand and predict the properties and transformations of molecules and materials. In particular, his theoretical advances have made possible dramatic advances in our understanding of the properties of novel nanoscale materials.

The theoretical advances by the nominee address the fundamental challenge of how quantum mechanics can be applied to realistic systems of molecules and solids in which the number of electrons in the system is very large and, particularly, to the question of how the excited states of these systems can be calculated and understood. These are deep theoretical challenges that have existed since the advent of quantum mechanics a century ago. The challenges are one with great practical implications for the development of new nanomaterials for information technology, medicine, and energy. By his successful development of new theoretical methodologies, Prof. Louie has opened the door to understanding the excited-state properties of a wide variety of new materials, including important nanoscale systems like carbon nanotubes, graphene, and novel two-dimensional materials.

Density functional theory, based on the Hohenberg-Kohn theorems, provides a method of handling the complex many-body interactions of real materials within a rigorous and computationally tractable framework. This type of method, however, is not suitable for a determination of the excited-state properties. In addition to the fundamental scientific importance of excited states, these states provide a key probe of material properties through spectroscopic signatures, determine properties of optical detectors, emitters, and energy-harvesting systems, and define photo-induced reactions and transformations.

Prof. Steven Louie pioneered the rigorous calculation of excited states in bulk and nanoscale materials. The method is based on his systematic development of many-body perturbation theory to take into account strong electron-electron interactions. The resulting *ab initio* GW-method, together with its realization in efficient codes, has had a dramatic impact on our ability to predict the properties of a wide range of materials.

Prof. Louie's research is universally recognized as defining and advancing the state of the art in electronic structure calculations and the understanding of excited states. The impact of Prof. Louie's research can easily be seen in the 85,000+ citations that his papers have received. In view of the ever-advancing computational capabilities available to researchers across the globe, the impact of Prof. Louie's research advances continues to grow.

I personally have benefitted enormously from the insights that Prof. Louie and his students have obtained into the properties of excitations in nanoscale materials. His research group was responsible for the quantitative understanding of the optically excited excitonic states in the model one-dimensional system of carbon nanotubes. His work demonstrated that the inhomogeneous dielectric environment that carriers experience in carbon nanotubes gives rise to pronounced non-local screening effects, the consequence of which is a strong modification of the effective electron-hole interaction. This leads to dramatic changes in the spectrum of excited excitonic states and in the exciton binding energy compared to what simple, idealized models had predicted. These studies played a direct role in our understanding of experimental investigations in our group.

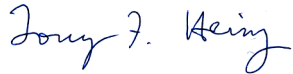
In the burgeoning field of two-dimensional materials, Prof. Louie's group was able to predict the absorption spectrum of the prototype material of graphene over a broad spectral range with great accuracy from purely *ab-initio* techniques. Prof. Louie was also able explain in detail how screening effects from free carriers acted to modify this spectrum, both through their screening of many-body interactions and through their creation of new inelastic relaxation pathways. This research was critical for extracting physical insight from our hard-won experimental data and provided important new insights into excited-state properties of this model 2D material. This research formed the basis of a very fruitful and important collaboration with our group, in which Prof. Louie's theoretical advances revealed the physical origin of the unexpected behavior that we saw in our measurements.

Prof. Louie's contributions to understanding the emerging properties of 2D semiconductors, such as the transition metal dichalcogenides, have been no less important for the interpretation of experimental findings of different research teams. In this area, his theoretical insight was also critical for our understanding of the fundamental properties of the materials determining their efficiency as novel light emitters for applications from lighting to medical probes.

Although these topics represent only a very small sampling of Prof. Steven Louie's prodigious research accomplishments, they have had a major impact on the most exciting fields of nanoscience. They also embody the accuracy, timeliness, and deep physical insight that characterize all of Prof. Louie's scientific work, features that make him stand out a star within the research community and assure the lasting impact of his contributions.

In view of his fundamental contributions to our understanding of materials by theoretical advances and his development of theoretical methods adopted by researchers across the globe, Prof. Steven Louie is a perfect candidate for recognition at the highest level. It is accordingly my pleasure to endorse his nomination for the “Albert Einstein” World Award of Science in the strongest terms.

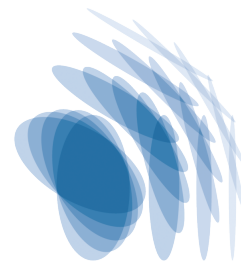
Yours sincerely,

A handwritten signature in blue ink that reads "Tony F. Heinz". The signature is written in a cursive, flowing style.

Tony F. Heinz
Professor of Applied Physics and Photon Science
Associate Laboratory Director, SLAC National Accelerator Laboratory

Max-Planck-Institut für Struktur und Dynamik der Materie

Max Planck Institute for the Structure and Dynamics of Matter



MPSD • Luruper Chaussee 149 • 22761 Hamburg

Albert Einstein World Award of Science
The World Cultural Council

Prof. Dr. Angel Rubio

Director
Theory Department
Luruper Chaussee 149
22761 Hamburg
Tel.: +49 40 8998 6550
angel.rubio@mpsd.mpg.de

Patricia Rihs, personal assistant
Tel.: +49 (0)40 8998 – 6555
Patricia.Rihs@mpsd.mpg.de

December 2nd, 2017

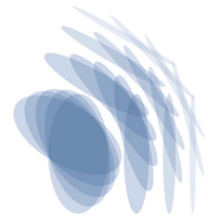
Dear Members of the panel for the Albert Einstein World Award of Science,

I am delighted to write this letter to support in the strongest terms possible the nomination of Prof. Steven G. Louie for the 2018 Albert Einstein World Award of Science. This conviction stems from Louie's seminal contributions to electronic structure theory, especially the development of unique first-principles methods for the prediction and understanding of ground and excited-state properties of many electron systems (solids, surfaces, nanostructures and molecules). In fact, Prof. Louie's is acknowledged worldwide as the pioneer and leader on the fundamentals of the theories behind today's first-principles density-functional frameworks to study a wide range of systems, from atoms, molecules to novel materials. Prof. Louie's far-reaching contributions have increased the basic knowledge and expanded the scope of chemical and materials science, and nanoscience over the past three decades. His work is and will remain a landmark for many scientific generations to come.

At the outset, I would like to address my eligibility to evaluate the capabilities of this remarkable scientist. I am a theoretical/computational chemist and physicist, who focuses primarily on laser-driven molecular excitations/ spectroscopy/dynamics, 2D molecular electronic spectroscopy, nanomaterials , molecular electronics/spintronics, electron/spin transport and molecular photonics. I am acknowledged as leader in the field of first-principles study of materials and electronic structure theory: including topical areas as graphene, carbon and BCN nanostructures, molecular junctions, complex and biological materials. I am the only Spanish Physics and Chemist appointed as Foreign Associate membership of the National Academy of Sciences (NAS) of United States, and this year I was awarded with the Max Born Medal and last year the Medal of the Royal Spanish Physical Society (2016) and in 2014 with the prestigious Jaime I prize for basic sciences as well as the DuPont Prize in Science 2006 and the Friedrich Wilhelm Bessel Research Award and the Royal Spanish Physics Society Prize. I am Fellow of the American Physical Society, American Association for the Advancement of Science (AAAS) and European Academia. As a world-leader scientist and close colleague of the nominee (and former postdoc), I would like to describe his qualification for the prize.

The impact of Louie's work on our basic understanding of the condensed matter is unrivaled in two ways: 1) they not only developed the central theoretical ideas but also invested enormous effort to implement them into computational tools which are now in widespread use



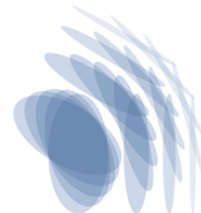


and which are essential in explaining and, moreover, predicting the behavior of broad classes of real materials, in particular low-dimensional materials and molecular nanostructures; and 2) he applied these methods to a wide variety of important examples, coming up with bold predictions that were later confirmed experimentally and powerful insights that advanced understanding of the fundamental behaviors of novel and complex nanostructures (e.g. nanotubes, graphene, atomically thin quasi-two-dimensional crystals, and many other related structures), enabling exploration of new directions and applications. According to the ISI he ranks among the most highly cited researchers in physics and materials science, illustrating the exceptional impact of Louie's work. Many of these studies are "firsts" and "new paradigms" that have greatly stimulated the development of the field and guided theoretical as well as experimental activities.

Recent experimental and theoretical studies of atomically thin quasi two-dimensional (2D) materials, such as graphene and monolayer or few-layer transition metal dichalcogenides TMDs (e.g., MoS_2 , MoSe_2 , WS_2 , WSe_2 , ...) and their nanostructures, have revealed that these systems can exhibit highly unusual behaviors. This field is currently one of the hottest and most rapidly developing areas of condensed matter physics and materials science, owing to its fundamental interest and great promise for applications. Professor Steven Louie has been leading the field, using electronic structure methods, to understand and predict some of the many novel electronic, transport and optical properties of these systems. His work has been extremely influential and impactful, both in terms of elucidating experimental observations and making discoveries/predictions of novel phenomena. Some of the topics he has unraveled are: satellite structures in photoemission of doped graphene (PRL 2013), atomic collapsed states in artificial nuclei on graphene (Science 2013), electron supercollimation in 2D Dirac fermion materials by disorder potentials (PRL 2014), tuning many-body interactions in electronic and optical properties of graphene via doping (PRL 2014), many-electron interactions and diversity of strongly bound excitons of different characters in the TMDs (PRL 2013), anomalous intrinsic quasi 2D screening and strong substrate effects in photophysics of the TMDs that lead to large bandgap renormalization and highly unusual bright/dark excitonic states which are non-hydrogenic-like and exhibit reversal of quantum level ordering (Nature 2014, Nature Materials 2014), and the evolution of interlayer coupling and electronic properties with geometry in twisted bilayer MoS_2 (Nature Commun. 2014), among others. In addition to their photophysics, Louie's group is now exploring a number of other phenomena in this class of materials -- tunable magnetism and half-metallicity, spatial indirect excitons and exciton condensations in layer heterojunctions, Coulomb drag effects, etc.

In addition I want to briefly highlight other very fundamental contributions of Prof. Louie in the context of the present nomination for the Buckley prize that has triggered a huge amount of research afterwards (as many of Prof. Louie's contributions). In the early 90's he predicted the existence and characterized the properties of novel carbon/boron/nitrogen nanotubes and related nanostructures leading to their ensuing experimental synthesis. This work has opened a new field of research in parallel to the one of carbon-based materials. He also developed the theory for understanding the unconventional mechanical properties of inorganic nanotubes (high Young's modulus, stiffness and flexibility) for applications in new high strength composite materials. In the early 2000's he discovered giant excitonic effects in both semiconducting and metallic carbon nanotubes, and in BN nanotubes. This prediction was met with some initial skepticism. Subsequent measurements however unambiguously demonstrated the existence and dominance of excitons, in full agreement with theory. Later on, he showed for the first time the phenomenon of "anti-screening" in nanotubes and other 1D/2D systems. In particular he predicted that graphene semiconducting nanoribbons with zigzag edges could be converted into half-metals applying an electric field. Moreover, he has demonstrated the importance of many-electron effects on the dramatic renormalization of molecular levels at metal-molecule interfaces. Inclusion of these effects is critical for the correct understanding of transport through single-molecule junctions.





Prof. Louie is having an enormous influence on both chemist and physics communities worldwide through his approach to science. He focuses on fundamental questions and very carefully develops the formalism that ultimately leads to novel computational techniques. In addition to his research accomplishments, Louie's manifold service on behalf of the scientific community are to be noted, inter alia as organizer or co-organizer of many international conferences and workshops. In addition to being a brilliant scientist, Steven Louie is also a great leader and teacher. In his lectures he is always careful to get the concepts across to his inspired audience. Moreover, he has trained generations of outstanding students and post-docs; many of them are now leading researchers in Europe, America, and Asia.

In summary, due to his outstanding accomplishments and impact and relevance of his work on low-dimensional materials and nanostructures I consider Prof. Louie the ideal candidate for the 2018 Albert Einstein World Award of Science.

Please do not hesitate to contact me if you need further comments or clarifications.

Sincerely

Prof. Dr. Ángel Rubio

Managing Director
Max Planck Institute for the Structure and Dynamics of Matter,
Hamburg, Germany



Statement of Achievements - Steven G. Louie for the 2018 Albert Einstein World Award of Science

Steven G. Louie is one of the most original and influential theorists in condensed matter and materials physics. He is a trailblazing leader who has advanced the frontiers of multiple fields across materials research by developing new concepts, pioneering critical theoretical and computational methods, predicting new properties and materials, providing insights to novel phenomena, and fostering interactions between theory and experiment. This nomination is to recognize his many seminal and far-reaching achievements, in particular in the quantum theory and computation of excited-state properties of matter, which have expanded the basic knowledge and shaped the scope of condensed matter physics, materials science, and nanoscience.

The impact of his work is unrivaled in two ways: 1) he not only developed the central ideas but also invested enormous effort to implement them into indispensable, powerful computational software that are in widespread use; and 2) he applied these methods to key problems, coming up with bold predictions and powerful insights that enabled exploration of new directions and applications.

Louie is the founder and acknowledged leader of the field of first-principles (i.e., without adjustable parameters or empirical input) study of electronic excited-state properties. Realizing the crucial importance of electron-electron interactions neglected in previous methods, he developed in 1985 an approach (based on the *GW* approximation of many-body theory) that allowed, for the first time, computation of electron excitation (quasiparticle) energies in real materials from *ab initio*. This breakthrough solved then a central problem in electronic structure theory (the bandgap problem) and created a vibrant field with worldwide following, complementing that of density functional theory (DFT) for ground-state properties. Later, in 1998, he included electron-hole interactions to his approach, making possible *ab initio* calculations (of unprecedented accuracy and predictability) of optical properties and related phenomena.

DFT-based methods have been very successful in analyzing the properties of solids from a total energy point of view, solving numerous important problems. But static DFT methods are rigorously unable to address electronic excited-state properties – e.g., bandgaps, band alignments at interfaces, tunneling and photoemission spectroscopies, optical excitations, etc. – with accuracy necessary to explain experiments or make predictions with confidence. Through the *ab initio* *GW* method and its extensions, Louie pioneered a powerful approach to address all of these challenging important issues. Without this approach, reliable predictions about the behavior of materials underlying electronic and optical applications would have been impossible. His body of work has transformed computational materials physics and spawned worldwide activities – leading to truly predictive results and novel insights on spectroscopic properties.

The impact and scope of Louie's methods were immediate upon development and have become even more apparent with time, in particular with the recent emphasis on nanoscience and energy research. His BerkeleyGW package, freely available to the community, is used by many groups worldwide. It is a petascale computing code that can address excited-state properties of systems with hundreds of atoms and scale up to >500,000 computer cores. A specific example is the establishment of the European Theoretical Spectroscopy Facility, which, to a large extent, is built on the powerful tools pioneered by Louie and collaborators.

Louie has made original scientific contributions of paramount importance to many different fields, and we turn to some highlights of his discoveries/achievements here. He is a world authority in the field of nanotubes. His seminal works include: prediction of new classes of nanotubes ($B_xC_yN_z$), concept of nanotubes (e.g., junctions) as nanodevices, understanding defects and external perturbations on their behaviors, prediction of giant excitonic effects in semiconducting and metallic nanotubes, discovery of “anti-screening” in nanotubes and other one-dimensional (1D) or two-dimensional (2D) systems, etc. Many of his studies, as his development of the *ab initio* *GW* method, are “firsts” and of “mind-changing” nature that shaped the field. For example, in 2003, Louie predicted from *ab initio* that the photophysics of semiconducting carbon nanotubes (CNTs) is totally dominated by excitons with huge binding energies

(fraction of an eV). This prediction was met with initial skepticism. Subsequent measurements unambiguously verified the existence and dominance of excitons in CNTs. He moreover first discovered that excitons exist even in metallic nanotubes, which have also been confirmed by experiment.

Louie has made numerous, groundbreaking advances in the rapidly developing field of atomically thin 2D crystals – graphene, transition metal dichalcogenides (TMDs), etc. – inspiring worldwide activities. He was first to predict from *ab initio* that graphene nanoribbons (GNRs) are semiconductors and that zigzag graphene nanoribbons may be made into half-metals with an electric field. His other “firsts” in this field include: discovery of anomalous dynamics and electron supercollimation of Dirac fermions in graphene superlattices and 1D disordered graphene; prediction of new generation massless Dirac fermions in graphene superlattices; creation of “artificial graphene” in patterned semiconductor 2D electron gas systems; prediction of strong excitonic effects in graphene and GNRs; elucidation of topological defects and novel transport through grain boundaries in graphene; discovery of topological phases in GNRs; etc.

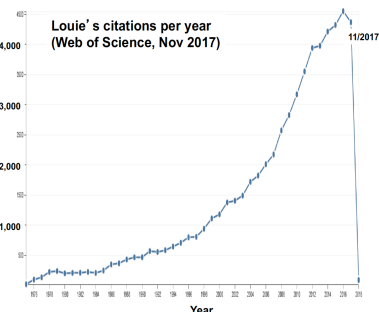
For mono- and few-layer 2D crystals, Louie’s *ab initio* work on the photophysics of MoS₂, MoSe₂, WS₂, WSe₂, GaSe, phosphorenes, etc. (e.g., predicting a diversity of strongly-bound bright and dark excitons that cannot be explained by conventional models) have stimulated many experimental studies worldwide that later confirmed his theoretical results. His other pioneering work in this area include the discoveries of massless excitons in monolayer TMDs, of tunable ferromagnetism in few-layer Cr₂Ge₂Te₆, and of magnetism and half-metallicity in hole-doped monolayer GaSe. Most recently, Louie discovered that band topological effects dramatically alter the optical selection rules for excitons in 2D crystals, and derived a *new* formula (involving a newly identified topological invariant) which generalizes, for the first time, the established selection rules that have been in use for the past six decades.

For single-molecule junctions, Louie first demonstrated the central importance of many-electron (self-energy) effects on renormalization of molecular levels at metal-molecule interfaces, an effect critical for the correct understanding of transport through single-molecule junctions.

Louie has been a towering figure in condensed matter physics and materials research for over 3 decades. In addition to the above highlights, in the 1970’s and 1980’s, he unraveled the properties of solids, surfaces and interfaces; developed a theory of Schottky barriers based on the metal-induced gap states; invented nonlinear pseudopotentials; pioneered *ab initio* methods for structural determination and phase transitions, as well as pioneered variational quantum Monte Carlo methods for real materials. Some of Louie’s other notable achievements include: invention of a formalism for computing NMR chemical shifts in solids and liquids; first-principles explanation of the multi-gap superconducting properties of MgB₂; discovery of an electronic mechanism for hardness; prediction of tunable spin polarization of photoelectrons from topological insulators; among others. He also developed a new Wannier-function-based method and code for electron-phonon interactions.

In short, Louie’s singularly influential body of breakthrough work in materials research has led to entirely new intuitions and inspired development of new fields, guiding new theoretical as well as experimental activities.

Louie has received many honors including election to the National Academy of Sciences and the American Academy of Arts & Sciences, as well as garnering of two major prizes from the American Physical Society (the Aneesur Rahman Prize and the Davisson-Germer Prize) and a major prize from the Materials Research Society (the Materials Theory Award). See his CV for a complete list. He is identified by *ISI Web of Science* (WoS) as a most highly cited researcher in physics – over 61,000 WoS citations with h-index of 120, and current yearly citations of over 4,500/year as of 11/2017 (over 80,000 citations and h-index of 140 on Google Scholar). See figure. He has trained generations of exceptional students and postdoctoral researchers; many are now leading scientists in the US, Europe, South America, and Asia.



Short Curriculum Vitae

Steven G. Louie

Professor of Physics, University of California at Berkeley
Senior Faculty Scientist, Lawrence Berkeley National Lab
Berkeley, California 94720, U.S.A.

Phone: (510) 642-1709

Email: sglouie@berkeley.edu

Homepage: <http://civet.berkeley.edu/louie>



PERSONAL DATA:

Born March 26, 1949, in Taishan, Guangdong, China; naturalized U.S. citizen, 1961; married with three children

EDUCATION:

- University of California at Berkeley, Ph.D. in Physics, 1976
- University of California at Berkeley, A.B. in Physics and Mathematics, 1972

SCIENTIFIC CAREER:

- Professor of Physics, University of California, Berkeley, 1984-present
- Founding Director, Center for Computational Study of Excited-State Phenomena in Energy Materials (C2SEPEM), Lawrence Berkeley National Laboratory, 2016-present
- Senior Faculty Scientist, Lawrence Berkeley National Laboratory, 1993-present
- Scientific Director, Theory Facility, the Molecular Foundry, 2001-2011
- Faculty Scientist, Lawrence Berkeley National Laboratory, 1981-93
- Associate Professor of Physics, University of California, Berkeley, 1980-84
- Assistant Professor of Physics, University of Pennsylvania, 1979-80
- Visiting Scientist, AT&T Bell Laboratories, Murray Hill, 1979
- Postdoctoral Fellow, I.B.M. Watson Research Center, 1977-79
- NSF Postdoctoral Fellow, University of California, Berkeley, 1976

SELECTED HONORS/AWARDS (reversed chronological order):

- H.C. Ørsted Lecturer, Technical University of Denmark, Denmark, 2017
- 2017 Jubilee Professorship, Chalmers University of Technology, Sweden, 2016
- Materials Theory Award of the Materials Research Society (MRS), 2015
- Inaugural Simons Fellow in Theoretical Physics, Simons Foundation, 2012
- Member, American Academy of Arts & Sciences, 2009
- Academician, Academia Sinica, Republic of China (Taiwan), 2008
- Mork Family Distinguished Lecturer, University of Southern California, 2008
- Distinguished Research Chair Professor, National Taiwan University, Taiwan, 2007-10
- Fellow, American Association for the Advancement of Science, 2006
- Closs Lecturer, University of Chicago, 2006
- Member, National Academy of Sciences, 2005
- Richard P. Feynman Prize in Nanotechnology (Theory), Foresight Institute, 2003
- Davisson-Germer Prize in Surface Physics, American Physical Society, 1999
- Aneesur Rahman Prize for Computational Physics, American Physical Society, 1996
- Sustained Outstanding Research in Solid State Physics Award, U.S. Dept of Energy, 1993
- Municipal Chair Professor, Joseph Fourier University, France, 1990
- John S. Guggenheim Foundation Fellow, 1989-90
- Eminent Visiting Scholar, University of Tokyo, 1989
- Professor, Miller Institute for Basic Research in Science, 1986-87, 1995
- Fellow, American Physical Society, 1985
- Alfred P. Sloan Foundation Fellow, 1980-82

PRINCIPAL RESEARCH INTERESTS

Theoretical condensed matter physics and nanoscience: electronic and structural properties of solids, surfaces, interfaces and clusters; quasiparticle and optical excitations; many-body effects in bulk and reduced-dimensional systems; graphene and graphene nanoribbons; carbon and BN nanotubes; quasi-2D materials beyond graphene; superconductivity; topological phases in matter; electron transport through nanostructures.

SCHOLARLY CONTRIBUTIONS

- More than **600** scientific publications, with over **60,900** ISI Web of Science citations and an **h-index** of **120**, as of November 2017 (over **85,000** citations and **h-index** of **140** on Google Scholar). Yearly number of WofS citations is currently at >4,500/year.
- Identified by the ISI Web of Science as one of the most highly cited researchers in physics, and one of the 25 most highly cited authors in nanoscience.
- Publications include **11** *Nature*, **8** *Science*, **129** *Phys. Rev. Lett.*, **5** *Nature Phys.*, **5** *PNAS*, **3** *Nature Materials*, **7** *Nature Nanotech.*, **4** *Nature Commun.*, **26** *Nano Lett.*, **5** *ACS Nano*, **4** *Applied Phys. Lett.*, **232** *Phys. Rev. B* articles, etc.
- Awarded **7** U.S. patents
- Authored the textbook (with M.L. Cohen): *Fundamentals of Condensed Matter Physics* (Cambridge University, 2016). Co-editor of **3** additional books: *Quantum Theory of Real Materials* (Kluwer, 1996); *The Optical Properties of Materials*, MRS Symp. Proceed. Vol. 579 (MRS, 2000); *Conceptual Foundations of Materials: A Standard Model for Ground- and Excited-State Properties* (Elsevier, 2006).
- Originator of **3** widely-use *ab initio* computational materials software packages: the density functional theory code “PARATEC”, the many-body excited-state properties code “BerkeleyGW”, and the Wannier functions electron-phonon coupling code “EPW”. All are available freely to users worldwide.
- More than **500** invited talks at conferences, universities and research institutions.
- Supervised **36** PhD students and over **50** postdoctoral fellows.

SELECTED PROFESSIONAL AND SERVICE ACTIVITIES (SINCE 2005)

Professor Louie is the Founding Director of the Center for Computational Study of Excited-State Phenomena in Energy Materials (C2SEPEM) at LBNL. He was a founding scientific director of the Molecular Foundry until 2011, and an editor of *Solid State Communications*, 1994-2011. He served on numerous national/international committees, panels, and boards. Selected recent activities include: Executive Committee of the American Physical Society (APS) Div. of Materials Physics, 2005-08; APS Adler Award Committee, 2005; Visiting Committee, ISSP, U of Tokyo, 2005; Class Membership Committee, National Academy of Sciences (NAS), 2006-09; Organizer, U.S.-Taiwan Workshop on Nanoscience, 2006; Advisory Committee of the Inst. of Atomic and Molecular Sciences, Academia Sinica, Taiwan, 2007-2010, chair 2010-; Science Council, Asia Pacific Center for Theoretical Physics, Korea, 2009 -; Scientific Committee, Cariplo Foundation (Italy), 2009–2014; DOE-BES Review Panel, Ames National Lab, 2010; Physical Sciences Panel, Research Grants Council, Hong Kong, 2010 - 2017; Visiting Member, Inst. of Advanced Study, Hong Kong U of Science & Techn., 2011 -; Chair, NAS Class III International Temporary Nominating Group, 2011-; Organizer, 15th Intern. Conf. on Science and Application of Nanotubes (NT14), 2012–14; Senior Advisory Council, Molecular Foundry, LBNL, 2012–; Search Committee, President of Asian Pacific Center for Theoretical Physics, South Korea, 2012-2013; External Review Board, Area of Excellence Centers, Hong Kong, 2012–; DOE-BES Review Panel, Oak Ridge National Lab, 2012; NAS Baker Award Committee, 2013; Organizer, 17th Int. Workshop on Computational Physics & Materials Science, ICTP, Italy, 2015; Int. Scientific Advisory Board of the Institut Catala de Nanociencia i Nanotecnologia (ICN2), Spain, 2015-; Staff Committee, Materials Sciences Division, LBNL, 2016-; Chair, Int. Advisory Committee, Center for Theoretical and Computational Physics, University of Hong Kong, 2016-present; Int. Advisory Committee, National Center for Theoretical Sciences, Taiwan, 2016-present; External Visiting Committee, Department of Physics, Hong Kong Baptist University, Hong Kong, 2016; Search Committee, Director of Institute for Atomic and Molecular Sciences, Academia Sinica, Taiwan, 2016-17; Co-organizer, NSF-MolSSI Workshop on Materials Software, 2016-2017; Chair, Senior Staff Scientist Ad Hoc Review Committee, LBNL, 2017; among others.

Professor Steven G. Louie's List of 10 Most Important Papers for the 2017 Albert Einstein World Award of Science Nomination

The 10 publications below are selected from Professor Steven G. Louie's over 600 published papers. The numbers of citations indicated are from Google Scholar as of 12/07/2017; a complete list of his publications may be obtained on <http://civet.berkeley.edu/louie/publications/>

1. M. S. Hybertsen and **S. G. Louie**, "Electron Correlation in Semiconductors and Insulators: Band Gaps and Quasiparticle Energies," *Phys. Rev. B* **34**, 5390 (1986). [2,813 citations]
2. N. G. Chopra, R. J. Luyken, K. Cherrey, V. H. Crespi, M. L. Cohen, **S. G. Louie**, and A. Zettl, "Boron Nitride Nanotubes," *Science* **269**, 966 (1995). [2,752 citations]
3. M. Rohlfing and **S. G. Louie**, "Electron-hole Excitations and Optical Spectra from First Principles," *Phys. Rev. B* **62**, 4927 (2000). [872 citations]
4. H. J. Choi, D. Roundy, H. Sun, M. L. Cohen, and **S. G. Louie**, "The Origin of the Anomalous Superconducting Properties of MgB₂," *Nature* **418**, 758 (2002). [901 citations]
5. C. D. Spataru, S. Ismail-Beigi, L. X. Benedict, and **S. G. Louie**, "Excitonic Effects and Optical Spectra of Single-Walled Carbon Nanotubes," *Phys. Rev. Lett.* **92**, 077402 (2004). [896 citations]
6. J. B. Neaton, M. S. Hybertsen, and **S. G. Louie**, "Renormalization of Molecular Electronic Levels at Metal-Molecule Interfaces," *Phys. Rev. Lett.* **97**, 216405 (2006). [599 citations]
7. Y.-W. Son, M. L. Cohen, and **S. G. Louie**, "Energy Gaps in Graphene Nanoribbons," *Phys. Rev. Lett.* **97**, 216803 (2006). [3,786 citations]
8. Y.-W. Son, M. L. Cohen, and **S. G. Louie**, "Half-metallic Graphene Nanoribbons," *Nature* **444**, 347 (2006). [3,213 citations]
9. D. Y. Qiu, F. H. da Jornada, and **S. G. Louie**, "Optical Spectrum of MoS₂: Many-body Effects and Diversity of Exciton States," *Phys. Rev. Lett.* **111**, 216805 (2013). [569 citations]
10. Z. L. Ye, T. Cao, K. O'Brien, H. Y. Zhu, X. B. Yin, Y. Wang, **S. G. Louie**, and X. Zhang, "Probing Excitonic Dark States in Single-layer Tungsten Disulphide," *Nature* **513**, 214 (2014). [350 citations]

PUBLICATIONS

Steven G. Louie

1. S. G. Louie and M. L. Cohen, "Electronic Structure of Cesium under Pressure," *Phys. Rev. B* **10**, 3237 (1974).
2. S. G. Louie, J. R. Chelikowsky, and M. L. Cohen, "Local-Field Effects in the Optical Spectrum of Silicon," *Phys. Rev. Lett.* **34**, 155 (1975).
3. M. Schlüter, J. R. Chelikowsky, S. G. Louie, and M. L. Cohen, "Self-Consistent Pseudopotential Calculations on Si(111) Unreconstructed and (2x1) Reconstructed Surfaces," *Phys. Rev. Lett.* **34**, 1385 (1975).
4. M. Schlüter, J. R. Chelikowsky, S. G. Louie, and M. L. Cohen, "Self-Consistent Pseudopotential Calculations for Si(111) Surfaces: Unreconstructed (1x1) and Reconstructed (2x1) Model Structures," *Phys. Rev. B* **12**, 4200 (1975).
5. J. R. Chelikowsky, M. Schlüter, S. G. Louie, and M. L. Cohen, "Self-Consistent Pseudopotential Calculation for the (111) Surface of Aluminum," *Solid State Comm.* **17**, 1103 (1975).
6. M. L. Cohen, M. Schlüter, J. R. Chelikowsky, and S. G. Louie, "Self-Consistent Pseudopotential Method for Localized Configurations: Molecules," *Phys. Rev. B* **12**, 5575 (1975).
7. S. G. Louie and M. L. Cohen, "Self-Consistent Pseudopotential Calculation for a Metal-Semiconductor Interface," *Phys. Rev. Lett.* **35**, 866 (1975). [Erratum: *Phys. Rev. Lett.* **36**, 173 (1976).]
8. S. G. Louie, M. Schlüter, J. R. Chelikowsky, and M. L. Cohen, "Self-Consistent Electronic States for Reconstructed Si Vacancy Models," *Phys. Rev. B* **13**, 1654 (1976).
9. S. G. Louie and M. L. Cohen, "Electronic Structure of a Metal-Semiconductor Interface," *Phys. Rev. B* **13**, 2461 (1976).
10. J. R. Chelikowsky, S. G. Louie, and M. L. Cohen, "Surface States and Metal Overlayers on the (110) Surface of GaAs," *Solid State Comm.* **20**, 641 (1976).
11. S. G. Louie, J. R. Chelikowsky, and M. L. Cohen, "Theory of Semiconductor Surface States and Metal-Semiconductor Interfaces," *J. Vac. Sci. Technol.* **13**, 790 (1976).
12. S. G. Louie, K. M. Ho, J. R. Chelikowsky, and M. L. Cohen, "Surface States on the (001) Surface of Nb," *Phys. Rev. Lett.* **37**, 1289 (1976).
13. J. R. Chelikowsky, S. G. Louie, and M. L. Cohen, "Relaxation Effects on the (110) Surface of GaAs," *Phys. Rev. B* **14**, 4724 (1976).
14. S. G. Louie, J. R. Chelikowsky, and M. L. Cohen, "Ionicity and the Theory of Schottky Barriers," *Phys. Rev. B* **15**, 2154 (1977).
15. M. L. Cohen and S. G. Louie, "Some Comments on the Excitonic Mechanism of Superconductivity," in *Superconductivity in d- and f-Band Metals*, ed. D. H. Douglass (Plenum Press, New York, 1976), p. 7.
16. K. M. Ho, S. G. Louie, J. R. Chelikowsky, and M. L. Cohen, "Self-Consistent Pseudopotential Calculation of the Electronic Structure of Nb," *Phys. Rev. B* **15**, 1755 (1977).
17. S. G. Louie and M. L. Cohen, "Superconducting Transition Temperatures for Weak and Strong Electron-Phonon Coupling," *Solid State Comm.* **22**, 1 (1977).

18. S. G. Louie, K. M. Ho, J. R. Chelikowsky, and M. L. Cohen, "Self-Consistent Pseudopotential Calculations for the Ideal (001) Surface of Nb," *Phys. Rev. B* **15**, 5627 (1977).
19. W. E. Pickett, S. G. Louie, and M. L. Cohen, "The Ge-GaAs (110) Interface: A Self-Consistent Calculation of Interface States and Electronic Structure," *Phys. Rev. Lett.* **39**, 109 (1977).
20. G.P. Kerker, S. G. Louie, and M. L. Cohen, "Electronic Structure of the Ideal and Reconstructed Si(001) Surface," *Phys. Rev. B* **17**, 706 (1978).
21. W. E. Pickett, S. G. Louie, and M. L. Cohen, "Self-Consistent Calculation of Interface States and Electronic Structure of the (110) Interfaces of Ge-GaAs and AlAs-GaAs," *Phys. Rev. B* **17**, 815 (1978).
22. J. Ihm, S. G. Louie, and M. L. Cohen, "Self-Consistent Pseudopotential Calculations for Ge and Diamond (111) Surfaces," *Phys. Rev. B* **17**, 769 (1978).
23. S. G. Louie and M. L. Cohen, "Dielectric Screening and Zone-Center Phonons in Si," *Phys. Rev. B* **17**, 3174 (1978).
24. J. Ihm, S. G. Louie, and M. L. Cohen, "Diamond-Metal Interfaces and the Theory of Schottky Barriers," *Phys. Rev. Lett.* **40**, 1208 (1978).
25. S. G. Louie, "Electronic States and Adsorbate-Induced Photoemission Structure on the Pd(111) Surface," *Phys. Rev. Lett.* **40**, 1525 (1978).
26. J. Ihm, S. G. Louie, and M. L. Cohen, "The Electronic Structure of Ge and Diamond Schottky Barriers," *Phys. Rev. B* **18**, 4172 (1978).
27. A. Pinczuk, S. G. Louie, B. Welber, J. C. Tsang, and J. A. Bradley, "The Conduction Band Parameters of GaAs at the D_{1C} Minima," in *Proceedings of the 14th International Conference on the Physics of Semiconductors*, ed. B.L.H. Wilson (Inst. of Phys., 1981), p. 1191.
28. S. G. Louie, K. M. Ho, and M. L. Cohen, "Self-Consistent Mixed-Basis Approach to the Electronic Structure of Solids," *Phys. Rev. B* **19**, 1774 (1979).
29. S. G. Louie, "H on Pd(111): Self-Consistent Electronic Structure, Chemical Bonding, and Photoemission Spectra," *Phys. Rev. Lett.* **42**, 476 (1979).
30. S. G. Louie, P. Thiry, R. Pinchaux, Y. Petroff, D. Chandesris, and J. Lecante, "Periodic Oscillations of the Frequency-Dependent Photoelectric Cross-Sections of Surface States: Theory and Experiment," *Phys. Rev. Lett.* **44**, 549 (1980).
31. S. G. Louie, "Cancellation Effects in Localized Orbital Theory," *Solid State Comm.* **34**, 723 (1980).
32. S. G. Louie, "New Localized Orbital Method for Calculating the Electronic Structure of Molecules and Solids: Covalent Semiconductors," *Phys. Rev. B* **22**, 1933 (1980).
33. S. G. Louie, "Electronic Structure of d-Band Metal Surfaces and Adsorption Systems," in *Physics of Transition Metals, 1980* (Proc. of the 2nd Conf. on the Physics of Transition Metals, Conf. Series No. 55), ed. P. Rhodes (Inst. of Physics, London, 1981), p. 401.
34. N.A.W. Holzwarth, S. G. Louie, and S. Rabii, "Electronic Structure of Third-Stage Lithium Intercalated Graphite," *Phys. Rev. Lett.* **47**, 1318 (1981).

35. Z. H. Levine and S. G. Louie, "New Model Dielectric Function and Exchange-Correlation Potential for Semiconductors and Insulators," *Phys. Rev. B* **25**, 6310 (1982).
36. S. G. Louie, S. Froyen, and M. L. Cohen, "Nonlinear Ionic Pseudopotentials in Spin Density Functional Calculations," *Phys. Rev. B* **26**, 1738 (1982).
37. N.A.W. Holzwarth, S. G. Louie, and S. Rabii, "X-Ray Form Factors and the Electronic Structure of Graphite," *Phys. Rev. B* **26**, 5382 (1982).
38. C. Minot and S. G. Louie, "Electronic Structure of Ditetramethyltetraselena-fulvalene-X [(TMTSF)₂X]: An Extended Hückel Calculation," *Phys. Rev. B* **26**, 4793 (1982).
39. S. G. Louie, "Calculated Optical and Photoemission Properties of GeSe₂," *Phys. Rev. B* **26**, 5993 (1982).
40. N.A. Holzwarth, S. G. Louie, and S. Rabii, "Electronic Structure of Graphite Intercalation Compounds," in *The Proceedings of the Symposium on Intercalated Graphite*, eds. M. S. Dresselhaus *et al.* (North Holland, New York, 1983), p. 107.
41. C. T. Chan and S. G. Louie, "Self-Consistent Pseudopotential Calculation of the Electronic Structure of PdH and Pd₄H," *Phys. Rev. B* **27**, 3325 (1983).
42. W. Eberhardt, S. G. Louie, and E.W. Plummer, "The Interaction of Hydrogen with a Pd(111) Surface," *Phys. Rev. B* **28**, 465 (1983).
43. N.A.W. Holzwarth, S. G. Louie, and S. Rabii, "Lithium Intercalated Graphite: Self-Consistent Electronic Structure for Stages One, Two, and Three," *Phys. Rev. B* **28**, 1013 (1983).
44. D. Vanderbilt and S. G. Louie, "A First Principles LCAO Study of Ideal and Reconstructed Diamond (111) 1×1 and 2×1 Surfaces," *J. Vac. Sci. and Techn.* **B1**, 723 (1983).
45. C. T. Chan and S. G. Louie, "Electronic Structure of Subsurface and Surface Chemisorption for Hydrogen on the Pd(111) Surfaces," *Solid State Comm.* **48**, 417 (1983).
46. J. R. Chelikowsky and S. G. Louie, "First Principles LCAO Method for the Cohesive and Structural Properties of Solids: Application to Diamond," *Phys. Rev. B* **29**, 3470 (1984).
47. D. Vanderbilt and S. G. Louie, "Total Energy Minimization for Diamond (111) Surfaces: Support for an Undimerized π -Bonded Chain Reconstruction," *Phys. Rev. B* **29**, 7099 (1984).
48. N.A.W. Holzwarth, S. G. Louie, and S. Rabii, "Theoretical Valence Charge Densities for Graphite, Diamond, and LiC₆," in *Local Density Approximations in Quantum Chemistry and Solid State Physics*, eds. J.P. Dahl and J. Avery (Plenum Press, New York, 1984), p. 665.
49. M. S. Hybertsen and S. G. Louie, "Non-Local Density Functional Theory for the Electronic and Structural Properties of Semiconductors," *Solid State Comm.* **51**, 451 (1984).
50. M. Y. Chou, S. G. Louie, M. L. Cohen, and N.A.W. Holzwarth, "Electron Momentum Distribution in Graphite and Lithium-Intercalated Graphite," *Phys. Rev. B* **30**, 1062 (1984).
51. N.A.W. Holzwarth, S. G. Louie, and S. Rabii, "Interlayer States in Graphite and in Alkali Metal-Graphite Intercalation Compounds," *Phys. Rev. B* **30**, 2219 (1984).
52. M. L. Cohen and S. G. Louie, "Electronic Properties of Surfaces," *Ann. Rev. Phys. Chem.* **35**, 537 (1984).

53. D. Vanderbilt, S. G. Louie, and M. L. Cohen, "Calculation of Phonon-Phonon Interactions and the Absence of Two-Phonon Bound States in Diamond," *Phys. Rev. Lett.* **53**, 1477 (1984).
54. D. Vanderbilt and S. G. Louie, "Total Energies of Diamond (111) Surface Reconstructions by an LCAO Method," *Phys. Rev. B* **30**, 6118 (1984).
55. C. T. Chan and S. G. Louie, "Hydrogen in Subsurface Sites of Pd(111): Self-Consistent Electronic Structure," *Phys. Rev. B* **30**, 4153 (1984).
56. D. Vanderbilt and S. G. Louie, "A Monte Carlo Simulated Annealing Approach to Optimization over Continuous Variables," *J. Comput. Phys.* **56**, 259 (1984).
57. J. R. Chelikowsky, S. G. Louie, D. Vanderbilt, and C. T. Chan, "Total Energy Method for Solids and Solid Surfaces," *Int. J. of Quant. Chem.: Quant. Chem. Symposium* **18**, 105 (1984).
58. M. S. Hybertsen and S. G. Louie, "Non-Local Density Functional Approximation for Exchange and Correlation in Semiconductors," *Phys. Rev. B* **30**, 5777 (1984).
59. S. G. Louie, "Pseudopotentials and Total Energy Calculations: Applications to Crystal Stability, Vibrational Properties, Phase Transformations, and Surface Structures," in *Proceedings of NATO International Advanced Study Institute on Electronic Structure, Dynamics, and Quantum Structural Properties of Condensed Matter*, eds. J. Devreese and P. Van Camp (Plenum Press, 1985), p. 335.
60. W. Maysenholder, S. G. Louie, and M. L. Cohen, "Cohesive Properties of bcc and fcc Rubidium from *ab initio* Pseudopotentials," *Phys. Rev. B* **31**, 1817 (1985).
61. M. Y. Chou, M. L. Cohen, and S. G. Louie, "Compton Profile of Graphite and Lithium-Intercalated Graphite," in *Proceedings of the Symposium on Intercalated Graphite Compounds*, eds. P.C. Eklund, M. S. Dresselhaus, and G. Dresselhaus (MRS, Pittsburgh, 1984), p.68.
62. M. Y. Chou, S. G. Louie, and M. L. Cohen, "Theoretical Study of Stacking Faults in Silicon," in *Proceedings of the 17th International Conference on the Physics of Semiconductors*, eds. D.J. Chadi and W. A. Harrison (Springer-Verlag, New York, 1985), p.43.
63. M. S. Hybertsen and S. G. Louie, "Calculation of Optical Gaps in Silicon in the Screened Exchange-Coulomb Hole Approximation," in *Proceedings of the 17th International Conference on the Physics of Semiconductors*, eds. D.J. Chadi and W. A. Harrison (Springer-Verlag, New York, 1985), p.1001.
64. M. Hanfland, K. Syassen, S. Fahy, S. G. Louie, and M. L. Cohen, "Pressure Dependence of the First-Order Raman Mode in Diamond," *Phys. Rev. B* **31**, 6896 (1985).
65. S. L. Richardson, M. L. Cohen, S. G. Louie, and J. R. Chelikowsky, "Comment on Predicted Modifications in the Direct and Indirect Gaps of Tetrahedral Semiconductors," *Phys. Rev. Lett.* **54**, 2549 (1985).
66. D. Vanderbilt and S. G. Louie, "Energy Minimization Calculations for Diamond (111) Surface Reconstructions," in *The Structure of Surfaces*, eds. M.A. Van Hove and S.Y. Tong (Springer-Verlag, New York, 1985), p.29.
67. S. G. Louie, "Total Energy Calculations and Bonding at Interfaces," *J. de Phys. Coll.* **C4**, 335 (1985).
68. S. B. Zhang, M. L. Cohen, and S. G. Louie, "Interface Potential Changes and Schottky Barriers," *Phys. Rev. B* **32**, 3955 (1985).
69. M. S. Hybertsen and S. G. Louie, "First Principles Theory of Quasiparticles: Calculation of Band Gaps in Semiconductors and Insulators," *Phys. Rev. Lett.* **55**, 1418 (1985).

70. M. S. Hybertsen and S. G. Louie, "Electron Correlation and the Band Gap in Ionic Crystals," *Phys. Rev. B* **32**, 7005 (1985).
71. M. Y. Chou, M. L. Cohen, and S. G. Louie, "Theoretical Study of Stacking Faults in Silicon," *Phys. Rev. B* **32**, 7979 (1985).
72. S. L. Richardson, M. L. Cohen, S. G. Louie, and J. R. Chelikowsky, "Electron Charge Densities at Conduction-Band Edges of Semiconductors," *Phys. Rev. B* **33**, 1177 (1986).
73. C. T. Chan, D. Vanderbilt, and S. G. Louie, "Application of a General Self-Consistent Scheme in the Linear Combination of Atomic Orbitals Formalism to the Electronic and Structural Properties of Si and W," *Phys. Rev. B* **33**, 2455 (1986). [Erratum: *Phys. Rev. B* **33**, 8791 (1986)].
74. C. T. Chan and S. G. Louie, "Theoretical Study of the Surface Energy and Surface Relaxation of W(001) Surface," *Phys. Rev. B* **33**, 2861 (1986). [Erratum: *Phys. Rev. B* **33**, 8792 (1986)].
75. M. Y. Chou, M. L. Cohen, and S. G. Louie, "Theoretical Compton Profiles of Graphite and LiC₆," *Phys. Rev. B* **33**, 6619 (1986).
76. D. Vanderbilt, S. G. Louie, and M. L. Cohen, "Calculation of Anharmonic Phonon Couplings in C, Si, and Ge," *Phys. Rev. B* **33**, 8740 (1986).
77. C. T. Chan, D. Vanderbilt, S. G. Louie, and J. R. Chelikowsky, "Theoretical Study of the Cohesive and Structural Properties of Mo and W in bcc, fcc, and hcp Structures," *Phys. Rev. B* **33**, 7941 (1986).
78. M. Hanfland, K. Syassen, S. Fahy, S. G. Louie, and M. L. Cohen, "The First-Order Raman Mode of Diamond under Pressure," *Physica* **139** and **140** B, 516 (1986).
79. S. B. Zhang, M. L. Cohen, and S. G. Louie, "Structural and Electronic Properties of the Al-GaAs(110) Interface," *Phys. Rev. B* **34**, 768 (1986).
80. S. Fahy, S. G. Louie, and M. L. Cohen, "Pseudopotential Total Energy Study of the Transition from Rhombohedral Graphite to Diamond," *Phys. Rev. B* **34**, 1191 (1986).
81. M. S. Hybertsen and S. G. Louie, "Spin-Orbit Splitting in Semiconductors and Insulators from the *ab initio* Pseudopotential," *Phys. Rev. B* **34**, 2920 (1986).
82. M. S. Hybertsen and S. G. Louie, "Electron Correlation in Semiconductors and Insulators: Band Gaps and Quasiparticle Energies," *Phys. Rev. B* **34**, 5390 (1986).
83. J. R. Chelikowsky, C. T. Chan, and S. G. Louie, "Theoretical Study of the Electronic, Structural, and Cohesive Properties of Ruthenium," *Phys. Rev. B* **34**, 6656 (1986).
84. S. G. Louie, "Quasiparticle Energies in Semiconductors and Insulators," in *Proceedings of the 18th Conference on the Physics of Semiconductors*, ed. D. Engstrom (World Scientific, Singapore, 1987), p. 1095.
85. D. Tomanek, C. T. Chan, and S. G. Louie, "*Ab initio* Calculation of Coverage-Dependent Adsorption Properties of H on Pd(001)," *Phys. Rev. Lett.* **57**, 2594 (1986). [Erratum: *Phys. Rev. Lett.* **58**, 287 (1987)]
86. C. T. Chan, S. G. Louie, and J. C. Phillips, "Potential Fluctuations and Density of Gap States in Amorphous Semiconductors," *Phys. Rev. B* **35**, 2744 (1987).

87. M. S. Hybertsen and S. G. Louie, "Many-body Calculation of Surface States: As on Ge(111)," *Phys. Rev. Lett.* **58**, 1551 (1987).
88. M. S. Hybertsen and S. G. Louie, "*Ab initio* Static Dielectric Matrices from the Density Functional Approach I: Formulation and Application to Semiconductors and Insulators," *Phys. Rev. B* **35**, 5585 (1987).
89. M. S. Hybertsen and S. G. Louie, "*Ab initio* Static Dielectric Matrices from the Density Functional Approach II: Calculation of the Screening Response in Diamond, Si, Ge and LiCl," *Phys. Rev. B* **35**, 5602 (1987).
90. S. Fahy, K.J. Chang, S. G. Louie, and M. L. Cohen, "Pressure Coefficients of Band Gaps of Diamond," *Phys. Rev. B* **35**, 5856 (1987).
91. D. Tomanek, S. G. Louie, H. J. Mamin, D. W. Abraham, R. E. Thomson, E. Ganz, and J. Clarke, "Theory and Observation of Highly Asymmetric Atomic Structure in Scanning Tunneling Microscopy Images of Graphite," *Phys. Rev. B* **35**, 7790 (1987).
92. S. Fahy, S. G. Louie, and M. L. Cohen, "Theoretical Total Energy Study of the Transformation of Graphite into Hexagonal Diamond," *Phys. Rev. B* **35**, 7623 (1987).
93. S. Fahy and S. G. Louie, "High Pressure Structural and Electronic Properties of Carbon," *Phys. Rev. B* **36**, 3373 (1987).
94. S. G. Louie, "Theory of Quasiparticle Energies and Excitation Spectra of Semiconductors and Insulators," in *Electronic Band Structure and Its Applications*, ed. M. Yussouff (Springer-Verlag, Heidelberg, 1987), p. 93.
95. J. E. Northrup, M. S. Hybertsen, and S. G. Louie, "Theory of Quasiparticle Energies in Alkali Metals," *Phys. Rev. Lett.* **59**, 819 (1987).
96. S. G. Louie and M. S. Hybertsen, "Theory of Quasiparticle Energies: Band Gaps and Excitation Spectra in Solids," *Int. J. of Quant. Chem.: Quant. Chem. Symp.* **21**, 31 (1987).
97. S. G. Louie, "*Ab initio* Calculation of Ground- and Excited-State Properties of Surfaces," in *Proceedings of the Asia-Pacific Symposium on Surface Physics*, ed. Xie Xide (World Scientific, Singapore, 1987), p. 140.
98. M. S. Hybertsen and S. G. Louie, "Theory and Calculation of Quasiparticle Energies and Band Gaps," *Comments on Cond. Mat. Phys.* **13**, 223 (1987).
99. U. Walter, S. Fahy, A. Zettl, S. G. Louie, M. L. Cohen, P. Tejedor, and A. M. Stacy, "Probing Electronic Density of States and Magnetic Interactions at the Rare Earth Site in $\text{ErBa}_2\text{Cu}_3\text{O}_7$," *Phys. Rev. B* **36**, 8899 (1987).
100. M. S. Hybertsen and S. G. Louie, "Model Dielectric Matrices for Quasiparticle Self-Energy Calculations," *Phys. Rev. B* **37**, 2733 (1988).
101. R. S. Becker, B.S. Swartzentruber, J.S. Vickers, M. S. Hybertsen, and S. G. Louie, "Geometric and Local Electronic Structure of Si(111)-As," *Phys. Rev. Lett.* **60**, 116 (1988).
102. C. Kittel, S. Fahy, and S. G. Louie, "Magnetic Screening by a Thin Superconducting Surface Layer," *Phys. Rev. B* **37**, 642 (1988).
103. D. Tomanek, R. M. Wentzcovitch, S. G. Louie, and M. L. Cohen, "Calculation of Electronic and Structural Properties of BC_3 ," *Phys. Rev. B* **37**, 3134 (1988).

104. D. Tomanek and S. G. Louie, "First Principles Calculation of Highly Asymmetric Structure in Scanning Tunneling Microscopy Images of Graphite," *Phys. Rev. B* **37**, 8327 (1988).
105. S. G. Louie, "Calculating and Predicting the Properties of Materials," in *High Speed Computing: Scientific Applications and Algorithm Design*, ed. R. B. Wilhelmsen (University of Illinois Press, Urbana, 1988), p. 112.
106. S. B. Zhang, D. Tomanek, S. G. Louie, M. L. Cohen, and M. S. Hybertsen, "Quasiparticle Calculation of Valence Band Offset of AlAs-GaAs(001)," *Solid State Comm.* **66**, 585 (1988).
107. M. S. Hybertsen and S. G. Louie, "Theory of Quasiparticle Surface States in Semiconductor Surfaces," *Phys. Rev. B* **38**, 4033 (1988).
108. R. M. Wentzcovitch, M. L. Cohen, and S. G. Louie, "Comparative Study of the Density of States of Graphite and BC₃," *Phys. Lett. A* **131**, 457 (1988).
109. R. M. Wentzcovitch, M. L. Cohen, S. G. Louie, and D. Tomanek, " σ -States Contribution to the Conductivity of BC₃," *Solid State Comm.* **67**, 515 (1988).
110. R. M. Wentzcovitch, S. Fahy, M. L. Cohen, and S. G. Louie, "*Ab initio* Study of Graphite Diamond-like Transitions in BN," *Phys. Rev. B* **38**, 6191 (1988).
111. S. Fahy, X. W. Wang, and S. G. Louie, "Variational Quantum Monte Carlo Non-Local Pseudopotential Approach to Solids: Cohesive and Structural Properties of Diamond," *Phys. Rev. Lett.* **61**, 1631 (1988).
112. M. Surh, J. E. Northrup, and S. G. Louie, "Occupied Quasiparticle Bandwidth of K," *Phys. Rev. B* **38**, 5976 (1988).
113. S. Fahy, C. Kittel, and S. G. Louie, "Electromagnetic Screening in Metals," *Am. J. Phys.* **56**, 989 (1988).
114. M. S. Hybertsen and S. G. Louie, "First-Principles Theory of Semiconductor Surface State Energies," in *Proceedings: 19th International Conference of the Physics of Semiconductors*, ed. W. Zawadzki (Inst. of Physics, Warsaw, Poland, 1988), Vol. I, p.713.
115. S. Fahy, X. W. Wang, and S. G. Louie, "Quantum Monte Carlo Calculation of the Properties of Atomic Carbon and Diamond," in *Proceedings: 19th International Conference of the Physics of Semiconductors*, ed. W. Zawadzki (Inst. of Physics, Warsaw, Poland, 1988), Vol. II, p.845.
116. M. F. Li, M.P. Surh, and S. G. Louie, "Spin-orbit Interaction Effects in Zincblende Semiconductors: *Ab Initio* Pseudopotential Calculations," in *Proceedings: 19th International Conference of the Physics of Semiconductors*, ed. W. Zawadzki (Inst. of Physics, Warsaw, Poland, 1988), Vol. II, p.857.
117. S. G. Louie, "First-Principles Calculation of Quasiparticle Energies at Surfaces and Interfaces: Semiconductor Surface-State Spectra and Band Offsets," in *Solvay Conference on Surface Science*, ed. F.W. de Wette (Springer-Verlag, Berlin, 1988), p. 399.
118. X. Zhu, S. Fahy, and S. G. Louie, "*Ab Initio* Calculation of Pressure Coefficients of Band Gaps of Silicon: Comparison of the LDA and Quasiparticle Results," *Phys. Rev. B* **39**, 7840 (1989). [Erratum: *B* **40**, 5821 (1989)]
119. S. G. Louie, "Variational Quantum Monte Carlo Calculation of Materials Properties," in *Atomic Scale Calculations in Materials Science*, Materials Research Society Symposium Proceedings, Vol. 141, eds. J. Tersoff *et al.* (MRS, Pittsburgh, 1989) p.3.

120. R. P. Andres, R. S. Averback, W. L. Brown, L. E. Brus, W. A. Goddard III, A. Kaldor, S. G. Louie, M. Moscovits, P. S. Peercy, S. J. Riley, R.W. Siegel, F. Spaepen, and Y. Wang, "Research Opportunities on Clusters and Cluster-Assembled Materials," *J. Mat. Res.* **4**, 704 (1989).
121. J. E. Northrup, M. S. Hybertsen, and S. G. Louie, "Quasiparticle Excitation Spectrum for Nearly Free Electron Metals," *Phys. Rev. B*, **39**, 8198 (1989).
122. S. B. Zhang, D. Tomanek, M. L. Cohen, S. G. Louie, and M. S. Hybertsen, "Evaluation of Quasiparticle Energies for Semiconductors without Inversion Symmetry," *Phys. Rev. B* **40**, 3162 (1989).
123. S. Saito, S. B. Zhang, S. G. Louie, and M. L. Cohen, "Quasiparticle Energies in Small Metal Clusters," *Phys. Rev. B* **40**, 3643 (1989).
124. S. G. Louie, "Theory of Ground- and Excited-State Properties of Solids, Surfaces, and Interfaces: Beyond Density Functional Formalism," in *Atomistic Simulation of Materials*, eds. V. Vitek and D.J.Srolovitz (Plenum Press, New York, 1989), p.125.
125. X. W. Wang, S. G. Louie, and M. L. Cohen, "Hydrogen Interactions in PdH_n ($1 \leq n \leq 4$)," *Phys. Rev. B* **40**, 5822 (1989).
126. S. B. Zhang, M. S. Hybertsen, M. L. Cohen, S. G. Louie, and D. Tomanek, "Quasiparticle Band Gaps for Ultrathin GaAs/AlAs(001) Superlattices," *Phys. Rev. Lett.* **63**, 1495 (1989).
127. S. G. Louie, "Ab initio Calculation of Materials Properties," in *Proceedings of the DOE Workshop on Theory, Modeling and Instrumentation for Materials by Design*, eds. R. E. Allen *et al.* (Oak Ridge National Laboratory Conference Proceedings CONF-8409210, 1989), p.128.
128. X. Zhu, S. B. Zhang, S. G. Louie, and M. L. Cohen, "Quasiparticle Interpretation of Photoemission Spectra and Optical Properties of GaAs(110)," *Phys. Rev. Lett.* **63**, 2112 (1989).
129. X. W. Wang and S. G. Louie, "First Principles Studies of S/Mo(001) Surfaces," *Surf. Sci.* **226**, 257 (1990).
130. S. B. Zhang, M. L. Cohen, S. G. Louie, D. Tomanek, and M. S. Hybertsen, "Quasiparticle Band Offset at the (001) Interface and Band Gaps in Ultrathin Superlattices of GaAs-AlAs Heterojunctions," *Phys. Rev. B* **41**, 10058 (1990).
131. M. S. Hybertsen and S. G. Louie, "Self-Energy Approach to Quasiparticle Energies Using a Density Functional Treatment of Dielectric Screening," in *Density Functional Theory of Many-Fermion Systems*, ed. S. B. Trickey (1990), p. 155.
132. S. G. Louie, "Variational Quantum Monte Carlo Calculation of Electronic and Structural Properties of Crystals," in *Quantum Simulation of Condensed Matter Phenomena*, ed. J. Gubernatis (World Scientific, Singapore, 1990), p.168.
133. S. Fahy, X. W. Wang, and S. G. Louie, "Variational Quantum Monte Carlo Nonlocal Pseudopotential Approach to Solids: Formulation and Application to Diamond, Graphite, and Silicon," *Phys. Rev. B* **42**, 3503 (1990). Erratum: *Phys. Rev. B* **43**, 9299 (1991).
134. X. Zhu, S. B. Zhang, S. G. Louie, and M. L. Cohen, "Zhu *et al.* Reply to Anisotropy in the Optical Spectrum of the GaAs (110) Surface," *Phys. Rev. Lett.* **65**, 938 (1990).
135. S. Fahy, X. W. Wang, and S. G. Louie, "Pair-Correlation Function and Single-Particle Occupation Numbers in Diamond and Silicon," *Phys. Rev. Lett.* **65**, 1478 (1990).

136. T. Pang and S. G. Louie, "Negative Donor Centers in Semiconductors and Quantum Wells," *Phys. Rev. Lett.* **65**, 1635 (1990).
137. X. Zhu, M. S. Hybertsen, and S. G. Louie, "Theory of the Quasiparticle Effective Masses in Semiconductors Based on an Electron Self Energy Approach," *Mat. Res. Soc. Symp. Proc.* **193**, 113 (1990).
138. S. Saito, S. B. Zhang, S. G. Louie, and M. L. Cohen, "New Formalism for Determining Excitation Spectra of Many-body Systems," *Phys. Rev. B* **42**, 7391 (1990).
139. S. Saito, S. B. Zhang, S. G. Louie, and M. L. Cohen, "Quasiparticle Energies in Small Alkali-Metal Clusters," *J. Phys. Cond. Matt.* **2**, 9041 (1990).
140. X. W. Wang, J. Zhu, S. G. Louie, and S. Fahy, "Magnetic Structure and Equation of State of bcc Solid Hydrogen: A Variational Quantum Monte Carlo Study," *Phys. Rev. Lett.* **65**, 2414 (1990).
141. H. Chacham, X. Zhu, and S. G. Louie, "Metal-Insulator Transition in Solid Xenon at High Pressures," *Europhys. Lett.* **14**, 65 (1991).
142. H. Chacham and S. G. Louie, "Metallization of Solid Hydrogen at Megabar Pressures: A First-Principles Quasiparticle Study," *Phys. Rev. Lett.* **66**, 64 (1991).
143. J. E. Northrup, M. S. Hybertsen, and S. G. Louie, "Many-Body Calculation of the Surface State Energies for Si(111)2×1," *Phys. Rev. Lett.* **66**, 500 (1991).
144. M.P. Surh, M.-F. Li, and S. G. Louie, "Spin-Orbit Splitting of GaAs and InSb Bands near G," *Phys. Rev. B* **43**, 4286 (1991).
145. D. Tomanek, Z. Sun, and S. G. Louie, "*Ab initio* Calculation of Chemisorption Systems: H on Pd(001) and Pd(110)," *Phys. Rev. B* **43**, 4699 (1991).
146. L. C. Brunel, S. G. Louie, G. Martinez, S. Labdi, and H. Raffy, "Superconducting Gap in Bi₂Sr₂CaCu₂O₈," *Phys. Rev. Lett.* **66**, 1346 (1991).
147. X. W. Wang, S. G. Louie, and M. L. Cohen, "Predicting High Pressure and Excited State Properties of Real Materials," *Int. J. of Supercom. Applic.*, **5**, 21 (1991).
148. J. E. Northrup, M. S. Hybertsen, and S. G. Louie, "Many-Body Calculation of the Surface State Energies for Si(111)2×1," in *Proceedings of the 20th International Conference on the Physics of Semiconductors*, eds. E.M. Anastassakis and J.D. Joannopoulos (World Scientific, Singapore, 1990), p. 119.
149. M.P. Surh, S. G. Louie, and M. L. Cohen, "Quasiparticle Energies for Cubic BN, BP, and BAs," *Phys. Rev. B* **43**, 9126 (1991).
150. S. B. Zhang, M. L. Cohen, and S. G. Louie, "Chemical Shift and Zone-Folding Effects in the Energy Gaps of GaAs-AlAs(001) Superlattices," *Phys. Rev. B* **43**, 9951 (1991).
151. X. Zhu and S. G. Louie, "Quasiparticle Surface Band Structure and Photoelectric Threshold of Ge(111)-2×1," *Phys. Rev. B* **43**, 12146 (1991).
152. X. Zhu and S. G. Louie, "Quasiparticle Band Structure of Thirteen Semiconductors and Insulators," *Phys. Rev. B* **43**, 14142 (1991).
153. S. G. Louie, "Condensed Matter Physics," in *Yearbook of Science and the Future 1992* (Encyclopaedia Britannica, Inc., Chicago, 1991), p. 397.

154. S. G. Louie, "Theory of Electronic Excitations in Solids," in *Electronic Materials: A New Era of Materials Sciences*, eds. J. R. Chelikowsky and A. Franciosi (Springer-Verlag, Berlin, 1991), p. 23.
155. G. Martinez, L. C. Brunel, S. G. Louie, S. Labdi, and H. Rafty, "Superconducting Gap and Magnetic Field Effects in $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$," *Physica C* **185 - 189**, 1753 (1991).
156. S. G. Louie and T. Pang, "Negative Donor Centers in High Magnetic Fields and Quantum Wells," in *New Horizons in Low-Dimensional Electron Systems*, eds. H. Aoki *et al.* (Kluwer Press, 1992), p. 445.
157. S. G. Louie, "Ab initio Calculations of Properties of Crystals, Surfaces, and Materials under Pressure," in *Proceedings of the EOE First Energy Research Power Supercomputer Users Symposium*, (Oak Ridge National Laboratory Conference Proceedings, CONF-9105202), Section 14.
158. X. Zhu and S. G. Louie, "Anharmonicity of the Hydrogen-Carbon Stretch Mode on Diamond (111)- 1×1 ," *Phys. Rev. B* **45**, 3940 (1992).
159. X. Zhu, X. W. Wang, and S. G. Louie, "First-principles Pseudopotential Calculations of Magnetic Iron," *Phys. Rev. B* **45**, 8887 (1992).
160. M.P. Surh, S. G. Louie, and M. L. Cohen, "Band Gaps of Diamond under Anisotropic Stress," *Phys. Rev. B* **45**, 8239 (1992).
161. S. G. Louie, "Quasiparticle Excitations and Photoemission," in *Angle-Resolved Photoemission*, ed. S. D. Kevan (Elsevier, Amsterdam, 1992), p. 63.
162. S. G. Louie, "Theory of Electronic Excitations on Semiconductor Surfaces," *Appl. Surf. Sci.* **60/61**, 13 (1992).
163. H. Chacham, X. Zhu, and S. G. Louie, "Pressure-Induced Insulator-Metal Transitions in Solid Xenon and Hydrogen: A First-Principles Quasiparticle Study," *Phys. Rev. B* **46**, 6688 (1992).
164. A. García, C. Elsässer, X. Zhu, S. G. Louie, and M. L. Cohen, "On the Use of the Generalized Gradient Approximation in Total Energy Calculations for Solids," *Phys. Rev. B* **46**, 9829 (1992). [Erratum: *Phys. Rev. B* **47**, 4150 (1993).]
165. E. Shirley, X. Zhu, and S. G. Louie, "Core-Polarization in Semiconductors: Effects on Quasiparticle Energies," *Phys. Rev. Lett.* **69**, 2955 (1992).
166. X. -J. Zhu and S. G. Louie, "Wigner Crystallization in the Fractional Quantum Hall Regime: A Variational Quantum Monte Carlo Study," *Phys. Rev. Lett.* **70**, 335 (1993).
167. J. Zhu, S. G. Louie, and T. Pang, " D^- Centers in High Magnetic Fields and Quantum Wells," *Mat. Sci. Forum* **117 - 118**, 1 (1993).
168. K. Hricovini, R. Gunther, P. Thiry, A. Taleb-Ibrahimi, G. Indlekofer, J. E. Bonnet, P. Dumas, Y. Petroff, X. Blase, X. -J. Zhu, S. G. Louie, Y.J. Chabal, and P.A. Thiry "Electronic Structure and Its Dependence on Local Order for $\text{H}/\text{Si}(111)-(1\times 1)$ Surfaces," *Phys. Rev. Lett.* **70**, 1992 (1993).
169. S. G. Louie and X. -J. Zhu, "Electron Correlations in Semiconductors: Bulk Cohesive Properties and Magnetic-Field-Induced Wigner Crystal at Heterojunctions," in *Proceedings of the 21st International Conference on the Physics of Semiconductors*, eds. P. Jiang and H.-Z. Zheng (World Scientific, Singapore, 1992), p. 61.

170. X. -J. Zhu and S. G. Louie, "Quasiparticle Properties of Ge(111) 2×1 Surface," in *Proceedings of the 21st International Conference on the Physics of Semiconductors*, eds. P. Jiang and H.-Z. Zheng (World Scientific, Singapore, 1992), p. 493.
171. E. L. Shirley and S. G. Louie, "Electron Excitations in Solid C₆₀: Energy Gap, Band Dispersions, and Effects of Orientational Disorder," *Phys. Rev. Lett.* **71**, 133 (1993).
172. S. Huant, A. Mandray, J. Zhu, T. Pang, S. G. Louie, and B. Etienne, "Well-Width Dependence of D⁺ Cyclotron Resonance in Quantum Wells," *Phys. Rev. B* **48**, 2370 (1993).
173. L.-C. Brunel, S. G. Louie, G. Martinez, S. Labdi and H. Rafty, "Superconducting Gap in High T_c Superconductors: Bi₂Sr₂CaCuO₈," in *Proceedings of the International Conference on High Temperature Superconductivity and Localization Phenomena*, eds. A. A. Aronov, A. I. Larkin, and V. S. Lutovinov (World Scientific, Singapore, 1992), p. 279.
174. S. G. Louie, "Correlated Wavefunction Quantum Monte Carlo Approach to Solids," in *Interatomic Potential and Structural Stability*, eds. K. Terakura and H. Akai (Springer-Verlag, Berlin, 1993), p. 181.
175. R. Price, X. -J. Zhu, P.M. Platzman, and S. G. Louie, "Freezing of the Quantum Hall Liquid at $\nu = 1/7$ and $1/9$," *Phys. Rev. B* **48**, 11473 (1993).
176. A. Rubio, J.L. Corkill, M. L. Cohen, E. L. Shirley, and S. G. Louie, "Quasiparticle Band Structure of AlN and GaN," *Phys. Rev. B* **48**, 11810 (1993).
177. S. G. Louie, "Excited States in Electronic Structure Calculations," in Vacuum Ultraviolet Radiation Physics, *Proceedings of the 10th International VUV Conference*, eds. F.J. Wuilleumier, Y. Petroff, and I. Nenner, (World Scientific, Singapore), 1993, p.408.
178. X. -J. Zhu and S. G. Louie, "Spin-Ordering of Two-Dimensional Electron Lattices," *Phys. Rev. B* **48**, 13661 (1993).
179. S. G. Louie and E. L. Shirley, "Electron Excitation Energies in Fullerites: Many-Electron and Molecular Orientational Effects," *J. Phys. Chem. Solids* **54**, 1767 (1993).
180. T. Sasaki, A. M. Rappe, and S. G. Louie, "Application of Optimized Pseudopotentials to Magnetic Systems," *Science Reports of the Research Institute Tohoku University Series A - Physics, Chemistry, and Metallurgy*, Vol. **39**, 37 (1993).
181. S. G. Louie, "Quasiparticle Theory of Surface Electronic Excitation Energies," *Surf. Sci.* **299/300**, 346 (1994).
182. S. G. Louie and E. L. Shirley, "Quasiparticle Excitations and Photoemission Spectra in Solid C₆₀," *Brazilian Journal of Physics* **24**, 43 (1994).
183. X. Blase, X. -J. Zhu, and S. G. Louie, "Self-Energy Effects on the Surface State Energies of H-Si(111) 1×1," *Phys. Rev. B* **49**, 4973 (1994).
184. X. Blase, L. X. Benedict, E. L. Shirley, and S. G. Louie, "Hybridization Effects and Metallicity in Small Radius Carbon Nanotubes," *Phys. Rev. Lett.* **72**, 1878 (1994).
185. Y. Miyamoto, A. Rubio, M. L. Cohen, and S. G. Louie, "Chiral Tubules of Hexagonal BC₂N," *Phys. Rev. B* **50**, 4976 (1994).

186. X. Blase, A.J. R. da Silva, X. Zhu, and S. G. Louie, "Si 2p Core Level Chemical Shifts at the H/Si(111)-(1×1) Surface," *Phys. Rev. B (RC)*, **50**, 8102 (1994).
187. J. A. Carlisle, L.J. Terminello, A.V. Hamza, E.A. Hudson, E. L. Shirley, F.J. Himpsel, D.A. Lapiano-Smith, J.J. Jia, T.A. Callcott, R.C.C. Perera, D.K. Shuh, S. G. Louie, J. Stöhr, M.G. Samant, and D.L. Ederer, "Occupied and Unoccupied Orbitals of C₆₀ and C₇₀," *Mol. Cryst. and Liq. Cryst.* **256**, 819 (1994).
188. O. Zakharov, A. Rubio, X. Blase, M. L. Cohen, and S. G. Louie, "Quasiparticle Band Structures of Six II-VI Compounds: ZnS, ZnSe, ZnTe, CdS, CdSe, CdTe," *Phys. Rev. B* **50**, 10780 (1994).
189. S. G. Louie, "Electronic Structure of C₆₀ Fullerites and Nanotubes," in *Proc. Int. Conf. on Electronic Properties of Novel Materials - Progress in Fullerene Research*, eds. H. Kuzmany et al. (World Scientific, Singapore, 1994) p. 303.
190. X. Blase, A. Rubio, S. G. Louie, and M. L. Cohen, "Stability and Band Gap Constancy of Boron-Nitride Nanotubes," *Euro. Phys. Lett.* **28**, 335 (1994).
191. Y. Miyamoto, A. Rubio, S. G. Louie and M. L. Cohen, "Electronic Properties of Tubule Forms of Hexagonal BC₃," *Phys. Rev. B* **50**, 18360 (1994).
192. J. A. Carlisle, L.J. Terminello, E.A. Hudson, E. L. Shirley, F.J. Himpsel, J.J. Jia, T.A. Callcott, R.C.C. Perera, S. G. Louie, J. Stöhr, M.G. Samant, and D.L. Ederer, "Occupied and Unoccupied Orbitals of C₆₀ and C₇₀ Probed With C 1S Emission and Absorption," *Mat. Res. Soc. Symp. Proc.* **349**, 245 (1994).
193. B. Králik, A. M. Rappe, and S. G. Louie, "Correlated Wavefunction Monte Carlo Studies of Excitations in the Quantum Hall Liquids," in *Proc. of the 22nd International Conference on the Physics of Semiconductors*, 1994, ed. D.J. Lockwood, (World Scientific, Singapore, 1995), p.999.
194. C. Hartmann, M. Zigone, G. Martinez, E. L. Shirley, L. X. Benedict, S. G. Louie, M. S. Fuhrer, and A. Zettl, "Optical Investigation of the Electron-Phonon Interaction in C₆₀ Fullerites," in *Proc. of the 22nd International Conference on the Physics of Semiconductors*, 1994, ed. D.J. Lockwood, (World Scientific, Singapore, 1995), p.2105.
195. X. Blase, A. Rubio, S. G. Louie, and M. L. Cohen, "Quasiparticle Band Structure of Bulk Hexagonal Boron Nitride and Related Systems," *Phys. Rev. B* **51**, 6868 (1995).
196. Y. Miyamoto, A. Rubio, X. Blase, M. L. Cohen, and S. G. Louie, "Ionic Cohesion and Electron Doping of Thin Carbon Tubules with Alkali Atoms," *Phys. Rev. Lett.* **74**, 2993 (1995).
197. M.P. Surh, H. Chacham, and S. G. Louie, "Quasiparticle Excitation Energies for the F-Center Defect in LiCl," *Phys. Rev. B*, **51**, 7464 (1995).
198. Z. Weng-Sieh, K. Cherrey, N.S. Chopra, A. Zettl, R. Gronsky, X. Blase, Y. Miyamoto, A. Rubio, S. G. Louie, and M. L. Cohen, "Synthesis of B_xC_yN_z Nanotubes," *Phys. Rev. B (RC)* **51**, 11229 (1995).
199. R. P. Chin, X. Blase, Y. R. Shen, and S. G. Louie, "Anharmonicity and Lifetime of the CH Stretch Mode on Diamond H/C(111) - (1 x 1)," *Europhysics Lett.* **30**, 399 (1995).
200. N.G. Chopra, R.J. Luyken, K. Cherrey, V.H. Crespi, M. L. Cohen, S. G. Louie, and A. Zettl, "Boron-Nitride Nanotubes," *Science* **269**, 966 (1995).
201. X. -J. Zhu and S. G. Louie, "Variational Quantum Monte Carlo Study of Two-Dimensional Wigner Crystals: Exchange, Correlation, and Magnetic Field Effects," *Phys. Rev. B*, **52**, 5863 (1995).

202. X. Blase, A. Rubio, S. G. Louie, and M. L. Cohen, "A Mixed-Space Formalism for the Dielectric Response in Periodic Systems," *Phys. Rev. B* **52**, R 2225 (1995).
203. N.G. Chopra, L. X. Benedict, V.H. Crespi, M. L. Cohen, S. G. Louie, and A. Zettl, "Fully Collapsed Carbon Nanotubes," *Nature* **377**, 135 (1995).
204. C. Hartmann, M. Zigone, G. Martinez, E. L. Shirley, L. X. Benedict, S. G. Louie, M. S. Fuhrer, and A. Zettl, "Investigation of the Absorption Edge of C₆₀ Fullerite," *Phys. Rev. B* **52**, R 5550 (1995).
205. L. X. Benedict, S. G. Louie, and M. L. Cohen, "Static Polarizabilities of Single Wall Carbon Nanotubes," *Phys. Rev. B* **52**, 8541 (1995).
206. T. Sasaki, A. M. Rappe, and S. G. Louie, "*Ab Initio* Optimized Pseudopotential Calculation of Magnetic Systems," *Phys. Rev. B* **52**, 12760 (1995).
207. B. Králik, A. M. Rappe, and S. G. Louie, "Theory of the Spin-Flip Excitations in the $\nu=1$ Quantum Hall Liquid," *Phys. Rev. B* **52**, R 11626 (1995).
208. L. X. Benedict, V.H. Crespi, S. G. Louie, and M. L. Cohen, "Static Conductivity and Superconductivity of Carbon Nanotubes: Relations between Tubes and Sheets," *Phys. Rev. B* **52**, 14935 (1995).
209. Y. Miyamoto, M. L. Cohen, and S. G. Louie, "*Ab Initio* Calculation of Phonon Spectra for Graphite, BN and BC₂N Sheets," *Phys. Rev. B* **52**, 14971 (1995).
210. L. Chico, V.H. Crespi, L. X. Benedict, S. G. Louie, and M. L. Cohen, "Pure Carbon Nanoscale Devices: Nanotube Heterojunctions," *Phys. Rev. Letters* **76**, 971 (1996).
211. S. G. Louie, "Quasiparticle Theory of Electron Excitations in Solids," in *Quantum Theory of Real Materials*, eds. J. R. Chelikowsky and S. G. Louie, (Kluwer Press, Boston, 1996), p. 83.
212. E. L. Shirley and S. G. Louie, "Photoemission and Optical Properties of C₆₀ Fullerenes," in *Quantum Theory of Real Materials*, eds. J. R. Chelikowsky and S. G. Louie (Kluwer Press, Boston, 1996), p. 515.
213. A. Rubio, Y. Miyamoto, X. Blase, M. L. Cohen, and S. G. Louie, "Theoretical Study of One-Dimensional Chains of Metal Atoms in Nanotubes," *Phys. Rev. B* **53**, 4023 (1996).
214. Y. Miyamoto, S. G. Louie, and M. L. Cohen, "Chiral Conductivities of Nanotubes," *Phys. Rev. Lett.* **76**, 2121 (1996).
215. S. G. Louie, "Theoretical Study of the Structure and Electronic Properties of Carbon and B_xC_yN_z Nanotubes," in *The Chemical Physics of Fullerenes 10(5) Years Later*, ed. W. Andreoni (Kluwer Press, Boston, 1996), p. 419.
216. V.H. Crespi, L. X. Benedict, M. L. Cohen, and S. G. Louie, "Prediction of a Pure-Carbon Planar Covalent Metal," *Phys. Rev. B* **53**, 13303 (1996).
217. F. Mauri and S. G. Louie, "Magnetic Susceptibility of Insulators from First Principles," *Phys. Rev. Lett.* **76**, 4246 (1996).
218. A. Rubio, J. A. Alonso, X. Blase, L. C. Balbas, and S. G. Louie, "*Ab initio* Photoabsorption Spectra and Structures of Small Semiconductor and Metal Clusters," *Phys. Rev. Lett.* **77**, 247 (1996).
219. L. Chico, L. X. Benedict, S. G. Louie, and M. L. Cohen, "Quantum Conductance of Carbon Nanotubes with Defects," *Phys. Rev. B* **54**, 2600 (1996). [Erratum: **61**, 10511 (2000).]

220. F. Mauri, O. Zakharov, S. de Gironcoli, S. G. Louie, and M. L. Cohen, "Phonon Softening and Superconductivity in Tellurium under Pressure," *Phys. Rev. Lett.* **77**, 1151(1996).
221. S. G. Louie, "Ab Initio Calculation of Electron Excitation Energies in Solids," in *Modelling and Simulation for Materials Design*, eds. S. Nishijima and H. Onodera (NRIM, Japan, 1996) p. 61.
222. V.H. Crespi, N.G. Chopra, M. L. Cohen, A. Zettl, and S. G. Louie, "Anisotropic Electron Beam Damage and the Collapse of Carbon Nanotubes," *Phys. Rev. B* **54**, 5927 (1996).
223. E. L. Shirley, L. X. Benedict, and S. G. Louie, "Excitons in Solid C₆₀," *Phys. Rev. B* **54**, 10970 (1996).
224. S. G. Louie, "Nanoparticles Behaving Oddly," *Nature* **384**, 612 (1996).
225. L. X. Benedict, S. G. Louie, and M. L. Cohen, "Heat Capacity of Carbon Nanotubes," *Solid State Comm.* **100**, 177 (1996).
226. F. Mauri, B. G. Pfrommer, and S. G. Louie, "*Ab-Initio* Theory of NMR Chemical Shifts in Solids and Liquids," *Phys. Rev. Lett.* **77**, 5300 (1996).
227. B. G. Pfrommer, M. Côté, S. G. Louie, and M. L. Cohen, "Relaxation of Crystals with the Quasi-Newton Method," *J. Computational Physics* **131**, 233 (1997).
228. Y. Miyamoto, M. L. Cohen, and S. G. Louie, "Theoretical Investigation of Graphitic Carbon Nitride and Possible Tubule Forms," *Solid State Comm.* **102**, 605 (1997).
229. Y. A. Krotov, D.-H. Lee, and S. G. Louie, "Low Energy Properties of (n,n) Carbon Nanotubes," *Phys. Rev. Lett.* **78**, 4245 (1997).
230. S. G. Louie, "Structures and Properties of Carbon and B-C-N Nanotubes," in *Proceedings of the Robert A. Welch Foundation 40th Conference on Chemical Research: Chemistry on the Nanometer Scale* (The Robert A. Welch Foundation, Houston, 1997), p. 141.
231. K. Ohno, F. Mauri, and S. G. Louie, "Magnetic Susceptibility of Semiconductors by an All-electron First-Principles Approach," *Phys. Rev. B* **56**, 1009 (1997).
232. W. A. Caldwell, J.H. Nguyen, B. G. Pfrommer, F. Mauri, S. G. Louie, and R. Jeanloz, "Structure, Bonding, and Geochemistry of Xenon at High Pressures," *Science* **277**, 930 (1997).
233. B. Králik, A. M. Rappe, and S. G. Louie, "Variational Monte Carlo Calculation of the Spin Gap in the $\nu = 1$ Quantum Hall Liquid," *Phys. Rev. B* **56**, 4760 (1997).
234. S. Ogut, J. R. Chelikowsky, and S. G. Louie, "Quantum Confinement and Optical Gaps in Si Nanocrystals," *Phys. Rev. Lett.* **79**, 1770 (1997).
235. E. L. Shirley, X. -J. Zhu, and S. G. Louie, "Core Polarization in Solids: Formulation and Application to Semiconductors," *Phys. Rev. B* **56**, 6648 (1997).
236. B. G. Pfrommer, M. Côté, S. G. Louie, and M. L. Cohen, "*Ab Initio* Study of Silicon in the R8 Phase," *Phys. Rev. B* **56**, 6662 (1997).
237. F. Mauri, B. G. Pfrommer, and S. G. Louie, "Ab-initio NMR Chemical Shift of Diamond, Chemical-Vapor-Deposited Diamond, and Amorphous Carbon," *Phys. Rev. Lett.* **79**, 2340 (1997).

238. S. G. Louie, "First-Principles Theory of Electron Excitation Energies in Solids, Surfaces, and Defects," in *Topics in Computational Materials Science*, ed. C. Y. Fong (World Scientific, Singapore, 1997) p. 96.
239. O. Zakharov, M. L. Cohen, S. G. Louie, and D.R. Penn, "Dynamical Screening at the Metal-Semiconductor Interface and Excitonic Superconductivity," *J. of Phys. C: Cond. Matt.* **9**, 8501 (1997).
240. A. Rubio, J. A. Alonso, X. Blase, and S. G. Louie, "Theoretical Models for the Optical Properties of Clusters and Nanostructures," *Int. J. of Mod. Phys. B* **11**, 2727 (1997).
241. P. Delaney, H. J. Choi, J. Ihm, S. G. Louie, and M. L. Cohen, "Broken Symmetry and Pseudogaps in Ropes of Carbon Nanotubes," *Nature* **391**, 466 (1998).
242. S. Han, J. Ihm, S. G. Louie, and M. L. Cohen, "Enhancement of Surface Hardness: Boron on Diamond (111)," *Phys. Rev. Lett.* **80**, 995 (1998).
243. B. Králík, E. K. Chang, and S. G. Louie, "Structural Properties and Quasiparticle Band Structure of Zirconia," *Phys. Rev. B* **57**, 7027 (1998).
244. M. Rohlfing and S. G. Louie, "Excitonic Effects and the Optical Absorption Spectrum of Hydrogenated Si Clusters," *Phys. Rev. Lett.* **80**, 3320 (1998).
245. Y.-G. Yoon, B. G. Pfrommer, F. Mauri, and S. G. Louie, "NMR Chemical Shifts in Hard Carbon Nitride Compounds," *Phys. Rev. Lett.* **80**, 3388 (1998).
246. J. C. Grossman, M. Côté, S. G. Louie, and M. L. Cohen, "Electronic and Structural Properties of Molecular C₃₆," *Chem. Phys. Lett.* **284**, 344 (1998).
247. M. Rohlfing and S. G. Louie, "Quasiparticle Band Structure of HgSe," *Phys. Rev. B* **57**, R9392 (1998).
248. B. G. Pfrommer, S. G. Louie, and H. Simon, "Conjugate-Gradient Based Electronic Structure Calculations in the Cray T3E and SGI Power Challenge," *Proceedings Eighth SIAM Conference on Parallel Processing for Scientific Computing*
249. L. X. Benedict, N.G. Chopra, M. L. Cohen, A. Zettl, S. G. Louie, and V.H. Crespi, "Microscopic Determination of the Interlayer Binding Energy in Graphite," *Chem. Phys. Lett.* **286**, 490 (1998).
250. S. Ogut, J. R. Chelikowsky, and S. G. Louie, "Reply to a Comment on 'Quantum Confinement and Optical Gaps in Si Nanocrystals,'" *Phys. Rev. Lett.* **80**, 3162 (1998).
251. B. Králík, P. Delaney, and S. G. Louie, "Correlation Effects on the Compton Profile of Silicon," *Phys. Rev. Lett.* **80**, 4253 (1998).
252. C. Elsässer, J. Zhu, S. G. Louie, M. Fähnle, and C. T. Chan, "*Ab Initio* Study of Iron and Iron Hydride: I. Cohesion, Magnetism and Electronic Structure of Cubic Fe and FeH," *J. Phys.: Cond. Matt.* **10**, 5081 (1998).
253. C. Elsässer, Jing Zhu, S. G. Louie, B. Meyer, M. Fähnle, and C. T. Chan, "*Ab Initio* Study of Iron and Iron Hydride: II. Structural and Magnetic Properties of Close-Packed Fe and FeH," *J. Phys.: Cond. Matt.* **10**, 5113 (1998).
254. C. Elsässer, H. Krimmel, M. Fähnle, S. G. Louie, and C. T. Chan, "*Ab Initio* Study of Iron and Iron Hydride: III. Vibrational States of H Isotopes in Fe, Cr and Ni," *J. Phys.: Cond. Matt.* **10**, 5131 (1998).

255. M. Côté, J. C. Grossman, M. L. Cohen, and S. G. Louie, "Electron-Phonon Interactions in Solid C₃₆," *Phys. Rev. Lett.* **81**, 697 (1998).
256. M. Côté, J. C. Grossman, M. L. Cohen, and S. G. Louie, "Electronic, Structural and Superconducting Properties of Molecular and Solid C₃₆," in *Proceedings of the Symposium on: Recent Advances in the Chemistry and Physics of Fullerenes and Related Materials*, Vol. 6 (The Electrochemical Society, 1998) p. 33.
257. P. Delaney, B. Králik, and S. G. Louie, "Compton Profiles of Si: Pseudopotential Calculation and Reconstruction Effects," *Phys. Rev. B* **58**, 4320 (1998).
258. S. Saito, S. G. Louie, and M. L. Cohen, "Tight-Binding Formalism for Ionic Fullerides and Its Application to Alkali-C₆₀ Polymers," in *Mat. Res. Soc. Symp. Proc.* **491**, 395 (1998).
59. M. Côté, J. C. Grossman, M. L. Cohen, and S. G. Louie, "Theoretical Study of a New Three-Dimensional All-*sp*² Structure," *Phys. Rev. B* **58**, 664 (1998).
260. M. Rohlfing and S. G. Louie, "Electron-hole Excitations in Semiconductors and Insulators," *Phys. Rev. Lett.* **62**, 2312 (1998).
261. P. Cervantes, Q. Williams, M. Côté, M. Rohlfing, M. L. Cohen, and S. G. Louie, "Band Structures of CsCl-Structured BaS and CaSe at High Pressure: Implications for Metallization Pressures of the Alkaline Earth Chalcogenides," *Phys. Rev. B* **58**, 9793 (1998).
262. B. G. Pfroimmer and S. G. Louie, "Density-Functional Study of the Magnetic and Metal-Insulator Transition of bcc Hydrogen," *Phys. Rev. B* **58**, 12680 (1998).
263. M. S. Fuhrer, U. Varadarajan, W. Holmes, P.L. Richards, P. Delaney, S. G. Louie, and A. Zettl, "Transport and localization in single-walled carbon nanotubes," in *AIP Conference Proceedings* (no. 442), *Electronic Properties of Novel Materials - Progress in Molecular Nanostructures* (XI International Winterschool, Kirchberg Tyrol, Austria, March 1998) p. 69.
264. J. R. Chelikowsky, S. Ögüt, and S. G. Louie, "Optical Gaps and Screening in Quantum Dots," in *Computational Modeling and Simulation of Materials*, ed. P. Vincenzini (Proceedings of the 9th CIMTEC World Ceramic Congress and Forum on New Materials, 1999).
265. P.G. Collins, J. C. Grossman, M. Côté, M. Ishigami, C. Piskoti, S. G. Louie, M. L. Cohen, and A. Zettl, "Scanning Tunneling Spectroscopy of C₃₆," *Phys. Rev. Lett.* **82**, 165 (1999).
266. M. Rohlfing and S. G. Louie, "Optical Excitations in Conjugated Polymers," *Phys. Rev. Lett.* **82**, 1959 (1999).
267. J. C. Grossman, W. A. Lester, Jr., and S. G. Louie, "Cyclopentadiene Stability: Quantum Monte Carlo, Coupled Cluster, and Density Functional Theory Determinations," *Molecular Phys.* **96**, 629 (1999).
268. S. -H. Jhi, J. Ihm, S. G. Louie, and M. L. Cohen, "Electronic Mechanism of Hardness Enhancement in Transition-Metal Carbonitrides," *Nature* **399**, 132 (1999).
269. M. S. Fuhrer, W. Holmes, P.L. Richards, P. Delaney, S. G. Louie, and A. Zettl "Nonlinear Transport and Localization in Single-Walled Carbon Nanotubes," *Synthetic Met.* **103**, 2529 (1999).
270. M. Rohlfing and S. G. Louie, "Excitons and Optical Spectrum of the Si(111)-(2×1) Surface," *Phys. Rev. Lett.* **83**, 856 (1999).

271. S. Ögüt, J. R. Chelikowsky, and S. G. Louie, "Comment on 'Quantum Confinement and Optical Gaps in Si Nanocrystals' - Reply," *Phys. Rev. Lett.* **83**, 1270 (1999).
272. F. Mauri, B. G. Pfrommer, and S. G. Louie, "Signature of Surface States on NMR Chemical Shifts: A Theoretical Prediction," *Phys. Rev. B* **60**, 2941 (1999).
273. A. Mizel, L. X. Benedict, M. L. Cohen, S. G. Louie, A. Zettl, N.K. Budraa, and W.P. Beyermann, "Analysis of the Low-Temperature Specific Heat of Multiwalled Carbon Nanotubes and Carbon Nanotube Ropes," *Phys. Rev. B* **60**, 3264 (1999).
274. J. C. Grossman, A. Mizel, M. Côté, M. L. Cohen, and S. G. Louie, "Transition Metals and Their Carbides and Nitrides: Trends in Electronic and Structural Properties," *Phys. Rev. B* **60**, 6343 (1999).
275. J. C. Grossman, S. G. Louie, and M. L. Cohen, "Solid C₃₆: Crystal Structures, Formation, and Effects of Doping," *Phys. Rev. B Rapid Comm.* **60**, R6941 (1999).
276. P. Delaney, H. J. Choi, J. Ihm, S. G. Louie, and M. L. Cohen, "Broken Symmetry and Pseudogaps in Ropes of Carbon Nanotubes," *Phys. Rev. B* **60**, 7899 (1999).
277. M. Rohlfing and S. G. Louie, "Optical Reflectivity of the Si(111) - (2x1) Surface—The Role of the Electron-Hole Interaction," *Phys. Status Solid. A* **175**, 17 (1999).
278. Y. Miyamoto, A. Rubio, S. G. Louie and M. L. Cohen, "Self-inductance of Chiral Conducting Nanotubes," *Phys. Rev. B* **60**, 13885 (1999).
279. M. Rohlfing and S. G. Louie, "Quasiparticle and Optical Excitations in Solids and Clusters," *Electron Correlations and Materials Properties*, eds. A. Gonis, N. Kioussis, and M. Cifan (Kluwer Academic/Plenum, New York, 1999), p. 309.
280. H. J. Choi, J. Ihm, Y.-G. Yoon, and S. G. Louie. "Possible Explanation for the Conductance of a Single Quantum Unit in Metallic Carbon Nanotubes," *Phys. Rev. B* **60**, R14009 (1999).
281. P. L. McEuen, M. Bockrath, D. H. Cobden, Y.-G. Yoon, and S. G. Louie, "Disorder, Pseudospins, and Backscattering in Carbon Nanotubes," *Phys. Rev. Lett.* **83**, 5098 (1999).
282. B. G. Pfrommer, F. Mauri, and S. G. Louie, "NMR Chemical Shifts of Ice and Liquid Water: The Effects of Condensation," *J. Am. Chem. Soc.* **122**, 123 (2000).
283. A. Zettl, C. Piskoti, J. C. Grossman, M. L. Cohen, and S. G. Louie. "Effect of Alkali Doping on the Structural Stability of Solid C₃₆," in *AIP Conference Proceedings* (no. 486), *Electronic Properties of Novel Materials - Science and Technology of Molecular Nanostructures* (13th International Winterschool, Kirchberg, Austria, 27 Feb.-6 March 1999) p. 183.
284. J. C. Grossman, W. A. Lester, and S. G. Louie, "Quantum Monte Carlo and Density Functional Theory Characterization of 2-Cyclopentenone and 3-Cyclopentenone Formation from O(P-3) plus Cyclopentadiene," *J. Am. Chem. Soc.* **122**, 705 (2000).
285. M. L. Cohen, S. G. Louie, and A. Zettl, "Random Access of Nanodevices," *Solid State Comm* **113**, 549 (2000).
286. H. J. Choi, J. Ihm, S. G. Louie, and M. L. Cohen, "Defects, Quasibound States, and Quantum Conductance in Metallic Carbon Nanotubes," *Phys. Rev. Lett.* **84**, 2917 (2000).

287. M. S. Fuhrer, J. Nygard, L. Shih, M. Forero, Y.-G. Yoon, M. S. C. Mazzoni, H. J. Choi, J. Ihm, S. G. Louie, A. Zettl, and P. L. McEuen, "Crossed Nanotube Junctions," *Science* **288**, 494 (2000).
288. J. C. Grossman, C. Piskoti, S. G. Louie, M. L. Cohen, and A. Zettl, "Molecular and Solid C₃₆," in *Fullerenes: Chemistry, Physics, and Technology*, edited by K. M. Kadish and R. S. Ruoff (John Wiley & Sons, Inc., 2000), p. 887.
289. X. Blase, K. Lin, A. Canning, S. G. Louie, and D. C. Chrzan "Structure and Energy of the 90° Partial Dislocation in Diamond: A Combined Ab Initio and Elasticity Theory Analysis," *Phys. Rev. Lett.* **84**, 5780 (2000).
290. S. G. Louie, "Electronic Structure of Carbon and Boron-Carbon-Nitrogen Nanotubes," in *Fullerene-Based and Fullerene-Related Materials*, ed. W. Andreoni (Kluwer, Dordrecht, 2000), p. 381.
291. S. -H. Jhi, S. G. Louie, and M. L. Cohen, "Electronic Properties of Oxidized Carbon Nanotubes," *Phys. Rev. Lett.* **85**, 1710 (2000).
292. F. Mauri, A. Pasquarello, B. G. Pfrommer, Y.-G. Yoon, and S. G. Louie, "The Si-O-Si Bond Angle Distribution in Vitreous Silica from First-Principles ²⁹Si NMR Analysis," *Phys. Rev. B* **62**, R4786 (2000).
293. M. Rohlfing and S. G. Louie, "Electron-hole Excitations and Optical Spectra from First Principles," *Phys. Rev. B* **62**, 4927 (2000).
294. E. K. Chang, M. Rohlfing, and S. G. Louie, "Excitons and Optical Properties of Alpha-Quartz," *Phys. Rev. Lett.* **85**, 2613 (2000).
295. K. Bradley, S.H. Jhi, P.G. Collins, J. Hone, M. L. Cohen, S. G. Louie, A. Zettl, "Is the Intrinsic Thermoelectric Power of Carbon Nanotubes Positive?" *Phys. Rev. Lett.* **85**, 4361 (2000).
296. E. K. Chang, M. Rohlfing, and S. G. Louie, "First-Principles Study of Optical Excitations in Alpha-Quartz," in *The Optical Properties of Materials*, MRS Symp. Proceed. Vol. **579**, eds. E. L. Shirley, J. R. Chelikowsky, S. G. Louie, and G. Martinez (Materials Research Society, Warrendale, 2000), p. 3.
297. S. Ogut, J. R. Chelikowsky, and S. G. Louie, "Optical Properties of Silicon Nanocrystals: A First Principles Study," *The Optical Properties of Materials*, MRS Symp. Proceed. Vol. **579**, eds. E. L. Shirley, J. R. Chelikowsky, S. G. Louie, and G. Martinez (Materials Research Society, Warrendale, 2000), p. 81.
298. P.H. Zhang, V.H. Crespi, E. Chang, S. G. Louie, and M. L. Cohen, "Computational Design of Direct-Bandgap Semiconductors that Lattice-Match Silicon," *Nature* **409**, 69 (2001).
299. M. Rohlfing, M. L. Tiago, and S. G. Louie, "First-principles Calculation of Optical Absorption Spectra in Conjugated Polymers: Role of Electron-hole Interaction," *Synthetic Metals* **116**, 101 (2001).
300. J. C. Grossman, M. Rohlfing, L. Mitas, S. G. Louie, and M. L. Cohen, "High Accuracy Many-Body Computational Approaches for Excitations in Molecules," *Phys.Rev.Lett.* **86**, 472 (2001).
301. J. Lei, H. Sun, K.W. Yu, S. G. Louie, and M. L. Cohen, "Image Potential States on Periodically Corrugated Metal Surfaces," *Phys. Rev. B* **63**, 045408 (2001).
302. Y.-G. Yoon, M. S.C. Mazzoni, H. J. Choi, J. Ihm, and S. G. Louie, "Structural Deformation and Intertube Conductance of Crossed Carbon Nanotube Junctions," *Phys. Rev. Lett.* **86**, 688 (2001).

303. S. G. Louie, "Electron-hole Interaction and Optical Excitations in Solids, Surfaces, and Polymers," in *Proceedings of the 3rd Japan-Korea Joint Workshop on First-Principles Electronic Structure Calculations (JK2000)*, Tsukuba, Japan (2001), p. 77.
304. G. -M. Rignanese, X. Blase, and S. G. Louie, "Quasiparticle Effects on Tunneling Currents: A Study of C₂H₄ Adsorbed on the Si(001)-2x1 Surface," *Phys. Rev. Lett.* **86**, 2110 (2001).
305. S. -H. Jhi, S. G. Louie, M. L. Cohen, and J. Ihm "Vacancy Hardening and Softening in Transition Metal Carbides and Nitrides," *Phys. Rev. Lett.* **86**, 3348 (2001).
306. S. Ishii, K. Ohno, Y. Kawazoe, and S. G. Louie, "*Ab Initio* GW Quasiparticle Energies of Small Sodium Clusters by an All-Electron Mixed-Basis Approach," *Phys. Rev. B* **63**, 155104 (2001).
307. M. L. Tiago, E. K. Chang, M. Rohlfing, and S. G. Louie, "*Ab Initio* Study of Optical Absorption Spectra of Semiconductors and Conjugated Polymers," in *Proceedings of 25th International Conference on the Physics of Semiconductors*, eds. N. Miura and T. Ando (Springer-Verlag, Berlin, 2001), p.79.
308. Y.-H. Kim, K.J. Chang, and S. G. Louie, "Band-gap Modification by Radial Deformation in C, BN, and BC₃ Nanotubes," in *Proceedings of 25th International Conference on the Physics of Semiconductors*, eds. N. Miura and T. Ando (Springer-Verlag, Berlin, 2001), p. 1645.
309. Y.-H. Kim, K.J. Chang, and S. G. Louie, "Electronic Structure of Radially Deformed BN and BC₃ Nanotubes," *Phys. Rev. B.* **63**, 205408 (2001).
310. S. G. Louie, "*Ab Initio* Study of Optical Excitations: Role of Electron-hole Interaction," in *Conference Proceedings* (no. 577), *Density Functional Theory and Its Appl. to Materials*, eds. V.E. Van Doren, K. Van Alsenoy, and P. Geerlings (American Institute of Physics, Melville, N.Y. 2001), p. 151.
311. S. G. Louie, "Electronic Properties, Junctions, and Defects of Carbon Nanotubes," in *Carbon Nanotubes, Topics in Applied Physics* **80**, eds. M. S. Dresselhaus, G. Dresselhaus, and P. Avouris (Springer-Verlag, Heidelberg, 2001), p. 113.
312. S. -H. Jhi, S. G. Louie, M. L. Cohen, and J.W. Morris, Jr., "Mechanical Instability and Ideal Shear Strength of Transition Metal Carbides and Nitrides," *Phys. Rev. Lett.* **87**, 075503 (2001).
313. S. Ismail-Beigi, E. K. Chang, and S. G. Louie, "Coupling of Nonlocal Potentials to Electromagnetic Fields," *Phys. Rev. Lett.* **87**, 087402 (2001).
314. H. Sun, S. -H. Jhi, D. Roundy, M. L. Cohen, and S. G. Louie, "Structural Forms of Cubic BC₂N," *Phys. Rev. B* **64**, 094108 (2001).
315. Y.-G. Yoon and S. G. Louie, "Electronic Structure and Quantum Conductance of Carbon Nanotubes," in *Nanostructured Carbon for Advanced Applications*, eds G. Benedek et al (Kluwer,Dordrecht, 2001), p. 233.
316. E. K. Chang, X. Blase, and S. G. Louie, "Quasiparticle Band Structure of Lanthanum Hydride," *Phys. Rev. B* **64**, 155108 (2001).
317. S. G. Louie, "Electronic Structure and Quantum Conductance of Nanotube Structures: Defects, Crossed-Tube Junctions, and Nanopeapods," in *Nanonetwork Materials: Fullerenes, Nanotubes, and Related Systems*, ed. S. Saito et al, American Institute of Physics, 101 (2001).

318. C. D. Spataru, M.A. Cazalilla, A. Rubio, L. X. Benedict, P.M. Echenique, and S. G. Louie, "Anomalous Quasiparticle Lifetime in Graphite: Band Structure Effects," *Phys. Rev. Lett.* **87**, 246405 (2001).
319. P.H. Zhang, V.H. Crespi, E. Chang, S. G. Louie, and M. L. Cohen, "Theory of Metastable Group-IV Alloys Formed from CVD Precursors," *Phys. Rev. B* **64**, 235201 (2001).
320. J. C. Grossman, M.E. Colvin, N.L. Tran, S. G. Louie, and M. L. Cohen, "Aromaticity and Hydrogenation Patterns in Highly Strained Fullerenes," *Chem. Phys. Lett.* **356**, 247 (2002).
321. S. Ishii, K. Ohno, Y. Kawazoe, and S. G. Louie, "Ab Initio GW Quasiparticle Calculation of Small Alkali-Metal Clusters," *Phys. Rev. B* **65**, 245109 (2002).
322. B. Sadigh, T.J. Lenosky, M.-J. Caturla, A.A. Quong, L. X. Benedict, T. Diaz de la Rubia, M. M. Giles, M. Foad, C. D. Spataru, and S. G. Louie, "Large Enhancement of Boron Solubility in Silicon Due to Biaxial Stress," *Appl. Phys. Lett.* **80**, 4738 (2002).
323. H. J. Choi, D. Roundy, H. Sun, M. L. Cohen, and S. G. Louie, "First-Principles Calculation of the Superconducting Transition in MgB_2 within the Anisotropic Eliashberg Formalism," *Phys. Rev. B* **66**, 020513 (2002).
324. J. -L. Li, G. -M. Rignanese, E. K. Chang, X. Blase, and S. G. Louie, "GW Study of the Metal-Insulator Transition of bcc Hydrogen," *Phys. Rev. B* **66**, 035102 (2002).
325. H. J. Choi, D. Roundy, H. Sun, M. L. Cohen, and S. G. Louie, "The Origin of the Anomalous Superconducting Properties of MgB_2 " *Nature* **418**, 758 (2002).
326. Y.-G. Yoon, P. Delaney, and S. G. Louie, "Quantum Conductance of Multiwall Carbon Nanotubes," *Phys. Rev. B* **66**, 073407 (2002).
327. S. -H. Jhi, S. G. Louie, and M. L. Cohen, "Electronic Properties of Bromine-Doped Carbon Nanotubes," *Solid State Communications* **123**, 495 (2002).
328. L. X. Benedict, C. D. Spataru, and S. G. Louie, "Quasiparticle Properties of a Simple Metal at High Electron Temperatures," *Phys. Rev. B* **66**, 085116 (2002).
329. J. E. Northrup, M. L. Tiago, and S. G. Louie, "Surface Energetics and Growth of Pentacene," *Phys. Rev. B* **66**, 121404 (2002).
330. W. Luo, S. Ismail-Beigi, M. L. Cohen, and S. G. Louie, "Quasiparticle Band Structure of ZnS and ZnSe," *Phys. Rev. B* **66**, 195215 (2002).
331. V. Madhavan, T. Jamneala, K. Nagaoka, W. Chen, J.L. Li, S. G. Louie, and M. F. Crommie, "Observation of Spectral Evolution During the Formation of a Ni_2 Kondo Molecule," *Phys. Rev. B* **66**, 212411 (2002).
332. H. J. Choi, D. Roundy, H. Sun, M. L. Cohen, and S. G. Louie, "Superconductivity of MgB_2 from First-Principles," *CIMTEC 2002—3rd Forum on New Materials, 2nd International Conference "Computational Modelling and Simulation of Materials,"* eds. P. Vincenzini, A Lami (Techna, 2003), p. 15.
333. S. Ismail-Beigi and S. G. Louie, "Excited-State Forces within a First-Principles Green's Function Formalism," *Phys. Rev. Lett.* **90**, 076401 (2003).
334. H. J. Choi, M. L. Cohen, and S. G. Louie, "Anisotropic Eliashberg Theory of MgB_2 : T_c , Isotope Effects, Superconducting Energy Gaps, Quasiparticles, and Specific Heat," *Physica C* **385**, 66 (2003).

335. X. H. Lu, M. Grobis, K. H. Khoo, S. G. Louie, and M. F. Crommie, "Spatially Mapping the Spectral Density of a Single C₆₀ Molecule," *Phys. Rev. Lett.* **90**, 096802 (2003).
336. J. A. Alford, M. Y. Chou, E. K. Chang, and S. G. Louie, "First-principles Studies of Quasiparticle Band Structures of Cubic YH₃ and LaH₃," *Phys. Rev. B* **67**, 125110 (2003).
337. M. L. Tiago, J. E. Northrup, and S. G. Louie, "Ab Initio Calculation of the Electronic and Optical Properties of Solid Pentacene," *Phys. Rev. B* **67**, 115212 (2003).
338. W. L. Yang, V. Brouet, X.J. Zhou, H. J. Choi, S. G. Louie, M. L. Cohen, S.A. Kellar, P.V. Bogdanov, A. Lanzara, A. Goldoni, F. Parmigiani, Z. Hussain, and Z.-X. Shen, "Band Structure and Fermi Surface of Electron-Doped C₆₀ Monolayers," *Science* **300**, 303 (2003).
339. M. Cardona, M. L. Cohen, and S. G. Louie, "Leopoldo Máximo Falicov 1933–1995," *Biographical Memoirs* **83**, The National Academies Press, Washington, D.C. (2003), p. 3.
340. S. G. Louie, "Recollections of Walter Kohn," *Walter Kohn: Personal Stories and Anecdotes Told by Friends and Collaborators*, eds. M. Scheffler, P. Weinberger (Springer-Verlag, 2003), p. 138.
341. Y. G. Yoon, M. S.C. Mazzoni, and S. G. Louie, "Quantum Conductance of Carbon Nanotube Peapods," *Appl. Phys. Lett.* **83**, 5217 (2003).
342. M. Grobis, X. Lu, K. H. Khoo, S. G. Louie, and M. F. Crommie, "Energy Resolved Imaging of Fullerene Molecular Orbitals," *AIP Conference Proceedings* **696**, Issue 1 (2003), p.20.
343. H. Sun, F.J. Ribeiro, J. -L. Li, D. Roundy, M. L. Cohen, and S. G. Louie, "Ab initio Pseudopotential Studies of Equilibrium Lattice Structures and Phonons Modes of Bulk BC₃," *Phys. Rev. B* **69**, 024110 (2004).
344. H. J. Choi, D. Roundy, H. Sun, M. L. Cohen, and S. G. Louie, Reply to "Comment on 'First-principles Calculation of the Superconducting Transition in MgB₂ within the Anisotropic Eliashberg Formalism,'" *Phys. Rev. B* **69**, 056502 (2004).
345. C. D. Spataru, S. Ismail-Beigi, L. X. Benedict, and S. G. Louie, "Excitonic Effects and Optical Spectra of Single-Walled Carbon Nanotubes", *Phys. Rev. Lett.* **92**, 077402 (2004).
346. C. D. Spataru, S. Ismail-Beigi, L. X. Benedict, and S. G. Louie, "Quasiparticle Energies, Excitonic Effects and Optical Absorption Spectra of Small-diameter Single-walled Carbon Nanotubes," *Appl. Phys. A* **78**, 1129 (2004).
347. M. L. Tiago, S. Ismail-Beigi, and S. G. Louie, "Effect of Semicore Orbitals on the Electronic Band Gaps of Si, Ge, and GaAs Within the GW Approximation," *Phys. Rev. B* **69**, 125212 (2004).
348. K. H. Khoo, M. S.C. Mazzoni, and S. G. Louie, "Tuning the Electronic Properties of Boron Nitride Nanotubes with Transverse Electric Fields: A Giant DC Stark Effect," *Phys. Rev. B* **69**, 201401 (2004).
349. C. D. Spataru, L. X. Benedict, and S. G. Louie, "Ab Initio Calculation of Band-Gap Renormalization in Highly Excited GaAs," *Phys. Rev. B* **69**, 205204 (2004).
350. S. Saito, K. Umemoto, S. G. Louie, and M. L. Cohen, "Energetics and Structural Stability of Cs₃C₆₀," *Solid State Communications* **130**, 335 (2004).
351. Y. G. Yoon, B. G. Pfrommer, S. G. Louie, and A. Canning, "NMR Chemical Shifts in Amino Acids: Effects of Environments in the Condensed Phase," *Solid State Communications* **131**, 15 (2004).

352. P. Tangney, S. G. Louie, and M. L. Cohen, "Dynamic Sliding Friction Between Concentric Carbon Nanotubes," *Phys. Rev. Lett.* **93**, 065503 (2004).
353. P.H. Zhang, W.D. Luo, V.H. Crespi, M. L. Cohen, and S. G. Louie, "Doping Effects on the Electronic and Structural Properties of CoO_2 : An LSDA+U Study," *Phys. Rev. B* **70**, 085108 (2004).
354. X.H. Lu, M. Grobis, K. H. Khoo, S. G. Louie and M. F. Crommie, "Charge Transfer and Screening in Individual C_{60} Molecules on Metal Substrates: A Scanning Tunneling Spectroscopy and Theoretical Study," *Phys. Rev. B* **70**, 115418 (2004).
355. R.B. Capaz, C. D. Spataru, P. Tangney, M. L. Cohen, and S. G. Louie, "Hydrostatic Pressure Effects on the Structural and Electronic Properties of Carbon Nanotubes," *Phys. Status Solidi (b)* **241**, 3352 (2004).
356. M. Ishigami, H. J. Choi, S. Aloni, S. G. Louie, M. L. Cohen and A. Zettl, "Identifying Defects in Nanoscale Materials," *Phys. Rev. Lett.* **93**, 196803 (2004).
357. V. Brouet, W. L. Yang, X.J. Zhou, H. J. Choi, S. G. Louie, M. L. Cohen, A. Goldoni, F. Parmigiani, Z. Hussain and Z.X. Shen, "Orientation-Dependent C_{60} Electronic Structures Revealed by Photoemission Spectroscopy," *Phys. Rev. Lett.* **93**, 197601 (2004). [Erratum: *Phys. Rev. Lett.* **95**, 099903 (2005).]
358. M. L. Tiago, M. Rohlfing and S. G. Louie, "Bound Excitons and Optical Properties of Bulk *Trans*-Polyacetylene," *Phys. Rev. B* **70**, 193204 (2004).
359. A. Trave, F.J. Ribeiro, S. G. Louie and M. L. Cohen, "Energetics and Structural Characterization of C_{60} Polymerization in BN and Carbon Nanopeapods," *Phys. Rev. B* **70**, 205418 (2004).
360. P.H. Zhang, W.D. Luo, S. G. Louie and M. L. Cohen, "Fermi Surface of Na_xCoO_2 ," *Phys. Rev. Lett.* **93**, 236402 (2004).
361. W.D. Luo, W. Duan, S. G. Louie and M. L. Cohen, "Structural and Electronic Properties of *n*-Doped and *p*-Doped SrTiO_3 ," *Phys. Rev. B* **70**, 214109 (2004).
362. R.B. Capaz, C. D. Spataru, P. Tangney, M. L. Cohen, and S. G. Louie, "Temperature Dependence of the Band Gap of Semiconducting Carbon Nanotubes," *Phys. Rev. Lett.* **94**, 036801 (2005).
363. M. L. Tiago, S. Ismail-Beigi, and S. G. Louie, "Photoisomerization of Azobenzene from First-Principles Constrained Density-Functional Calculations," *J. Chem. Phys.* **122**, 094311 (2005).
364. M. Grobis, K. H. Khoo, R. Yamachika, X. Lu, K. Nagaoka, S. G. Louie, M. F. Crommie, H. Kato and H. Shinohara, "Spatially Dependent Inelastic Tunneling in a Single Metallofullerene," *Phys. Rev. Lett.* **94**, 136802 (2005).
365. P.H. Zhang, R.B. Capaz, M. L. Cohen, and S. G. Louie, "Theory of Sodium Ordering in Na_xCoO_2 ," *Phys. Rev. B* **71**, 153102 (2005).
366. S.Y. Zhou, G-H. Gweon, C. D. Spataru, J. Graf, D.-H. Lee, S. G. Louie and A. Lanzara, "Coexistence of Sharp Quasiparticle Dispersion and Disorder Features in Graphite," *Phys. Rev. B* **71**, 161403 (2005).
367. S. -H. Jhi, D.J. Roundy, S. G. Louie, and M. L. Cohen, "Formation and Electronic Properties of Double-Walled Boron Nitride Nanotubes," *Solid State Communications* **134**, 397 (2005).
368. P.H. Zhang, S. G. Louie, and M. L. Cohen, "Nonlocal Screening, Electron-Phonon coupling, and Phonon Renormalization in Metals," *Phys. Rev. Lett.* **94**, 225502 (2005).

369. J.L. Li, G.M. Rignanese, and S. G. Louie, "Quasiparticle Energy Bands of NiO in the GW Approximation," *Phys. Rev. B* **71**, 193102 (2005).
370. R.B. Capaz, C. D. Spataru, P. Tangney, M. L. Cohen, and S. G. Louie, "Temperature and hydrostatic pressure effects on the band gap of semiconducting carbon nanotubes," 27th Conference on the Physics of Semiconductors, *AIP Conference Proceedings* **772**, 1047 (2005).
371. C. D. Spataru, S. Ismail-Beigi, L. X. Benedict, and S. G. Louie, "Excitonic Effects and Optical Spectra of Single-Walled Carbon Nanotubes," 27th Conference on the Physics of Semiconductors, *AIP Conference Proceedings* **772**, 1061 (2005).
372. S. G. Louie and A. Rubio, "Quasiparticle and Optical Properties of Solids and Nanostructures: The GW-BSE Approach," *Handbook of Materials Modeling*, ed. S. Yip (Springer, Dordrecht, The Netherlands, 2005), p. 215.
373. J.B. Neaton, K. H. Khoo, C. D. Spataru, and S. G. Louie, "Electronic Transport and Optical Properties of Carbon Nanostructures from First Principles," *Comp. Phys. Comm.* **169**, 1 (2005).
374. F.J. Ribeiro, J.B. Neaton, S. G. Louie, and M. L. Cohen, "Mechanism for biased-assisted indium mass transport on carbon nanotube surfaces," *Phys. Rev. B* **72**, 075302 (2005).
375. M. Grobis, K. H. Khoo, R. Yamachika, X. Lu, K. Nagaoka, S. G. Louie, H. Kato, H. Shinohara, and M. F. Crommie, "Spatially Dependent Inelastic Tunneling in Gd@C₈₂," XIX International Winterschool/Euroconference on Electronic Properties of Novel Materials, *AIP Conference Proceedings* **786**, 8 (2005).
376. R.B. Capaz, C. D. Spataru, P. Tangney, M. L. Cohen, and S. G. Louie, "Family behavior of the pressure and temperature dependences of the band gap of semiconducting carbon nanotubes," XIX International Winterschool/Euroconference on Electronic Properties of Novel Materials, *AIP Conference Proceedings* **786**, 411 (2005).
377. S. Ismail-Beigi and S. G. Louie, "Self-Trapped Excitons in Silicon Dioxide: Mechanism and Properties," *Phys. Rev. Lett.* **95**, 156401 (2005).
378. A. Wachowiak, R. Yamachika, K. H. Khoo, Y. Wang, M. Grobis, D.-H. Lee, S. G. Louie, and M. F. Crommie, "Visualization of the Molecular Jan-Teller Effect in an Insulating K₄C₆₀ Monolayer," *Science* **310**, 468 (2005).
379. P.T. Tangney, R.B. Capaz, C. D. Spataru, M. L. Cohen, and S. G. Louie, "Structural Transformations of Carbon Nanotubes under Hydrostatic Pressure," *Nano Lett.* **5**, 2268 (2005).
380. Y.-W. Son, J. Ihm, M. L. Cohen, S. G. Louie, and H. J. Choi, "Electrical Switching in Metallic Carbon Nanotubes," *Phys. Rev. Lett.* **95**, 216602 (2005).
381. S. -H. Jhi, S. G. Louie, and M. L. Cohen, "Reentrant Semiconducting Behavior of Zigzag Carbon Nanotubes at Substitutional Doping by Oxygen Dimers," *Phys. Rev. Lett.* **95**, 226403 (2005).
382. C. D. Spataru, S. Ismail-Beigi, R.B. Capaz, and S. G. Louie, "Theory and Ab Initio Calculation of Radiative Lifetime of Excitons in Semiconducting Carbon Nanotubes," *Phys. Rev. Lett.* **95**, 247402 (2005).
383. F.J. Ribeiro, P. Tangney, S. G. Louie, and M. L. Cohen, "Structural and Electronic Properties of Carbon in Hybrid Diamond-graphite Structures," *Phys. Rev. B* **72**, 214109 (2005).
384. C.H. Park, C. D. Spataru, and S. G. Louie, "Excitons and Many-Electron Effects in the Optical Response of Single-Walled Boron Nitride Nanotubes," *Phys. Rev. Lett.* **96**, 126105 (2006).

385. H. J. Choi, M. L. Cohen, and S. G. Louie, "Anisotropic Eliashberg Theory and the Two-Band Model for the Superconducting Properties of MgB_2 ," *Phys. Rev. B* **73**, 104520 (2006).
386. S. B. Cronin, Y. Yin, A. Walsh, R.B. Capaz, A. Stolyarov, P. Tangney, M. L. Cohen, S. G. Louie, A.K. Swan, M. S. Unlu, B.B. Goldberg, and M. Tinkham, "Temperature Dependence of the Optical Transition Energies of Carbon Nanotubes: The Role of Electron-Phonon Coupling and Thermal Expansion," *Phys. Rev. Lett.* **96**, 127403 (2006).
387. E.B. Barros, R.B. Capaz, A. Jorio, G.G. Samsonidze, A.G. Souza Filho, S. Ismail-Beigi, C. D. Spataru, S. G. Louie, G. Dresselhaus, and M. S. Dresselhaus, "Selection Rules for One- and Two-Photon Absorption by Excitons in Carbon Nanotubes," *Phys. Rev. B* **73**, 241406 (2006).
388. S.Y. Quek, J.B. Neaton, M. S. Hybertsen, E. Kaxiras, and S. G. Louie, "First-principles Studies of the Electronic Structure of Cyclopentene on Si(001): Density Functional Theory and GW Calculations," *Phys. Status Solidi (b)* **243**, 2048 (2006).
389. Y.Z. Ma, C. D. Spataru, L. Valkunas, S. G. Louie, and G.R. Fleming, "Spectroscopy of Zigzag Single-Walled Carbon Nanotubes: Comparing Femtosecond Transient Absorption Spectra with Ab Initio Calculations," *Phys. Rev. B* **74**, 085402 (2006).
390. S.Y. Zhou, G.-H. Gweon, J. Graf, A.V. Fedorov, C. D. Spataru, R.D. Diehl, Y. Kopelevich, D.-H. Lee, S. G. Louie, and A. Lanzara, "First Direct Observation of Dirac Fermions in Graphite," *Nature Phys.* **2**, 595 (2006).
391. S. G. Louie, "Predicting Materials and Properties: Theory of the Ground and Excited State," *Conceptual Foundations of Materials: A Standard Model for Ground- and Excited-State Properties*, vol. eds., S. G. Louie, M. L. Cohen (Elsevier, Amsterdam, 2006) p. 9.
392. R.B. Capaz, C. D. Spataru, S. Ismail-Beigi, and S. G. Louie, "Diameter and Chirality Dependence of Exciton Properties in Carbon Nanotubes," *Phys. Rev. B* **74**, 121401 (2006).
393. F. J. Ribeiro, P. Tangney, S. G. Louie and M. L. Cohen, "Hypothetical Hard Structures of Carbon with Cubic Symmetry," *Phys. Rev. B* **74**, 172101 (2006).
394. P. Tangney, M. L. Cohen, and S. G. Louie, "Giant Wave-Drag Enhancement of Friction in Sliding Carbon Nanotubes," *Phys. Rev. Lett.* **97**, 195901 (2006).
395. Y.-W. Son, M. L. Cohen, and S. G. Louie, "Half-Metallic Graphene Nanoribbons," *Nature* **444**, 347 (2006). [Corrigendum: *Nature* 446, 342 (2007)]
396. J.B. Neaton, M. S. Hybertsen, and S. G. Louie, "Renormalization of Molecular Electronic Levels at Metal-Molecule Interfaces," *Phys. Rev. Lett.* **97**, 216405 (2006).
397. Y.-W. Son, M. L. Cohen, and S. G. Louie, "Energy Gaps in Graphene Nanoribbons," *Phys. Rev. Lett.* **97**, 216803 (2006). [Erratum: *Phys. Rev. Lett.* **98**, 089901 (2007)]
398. T. Miyake, P.H. Zhang, M. L. Cohen, and S. G. Louie, "Quasiparticle Energy of Semicore d -electrons in ZnS: Combined LDA+ U and GW approach," *Phys. Rev. B* **74**, 245213 (2006).
399. F. Giustino, J. R. Yates, I. Souza, M. L. Cohen, and S. G. Louie, "Electron-Phonon Interaction via Electron and Lattice Wannier Functions: Superconductivity in Boron-Doped Diamond Reexamined," *Phys. Rev. Lett.* **98**, 047005 (2007).

400. I.H. Choi, P.Y. Yu, P. Tangney, and S. G. Louie, "Vibrational Properties of Single Walled Carbon Nanotubes under Pressure from Raman Scattering Experiments and Molecular Dynamics," *Phys. Status Sol. (b)* **244**, 121 (2007).
401. S.Y. Quek, J.B. Neaton, M. S. Hybertsen, E. Kaxiras, and S. G. Louie, "Negative Differential Resistance in Transport through Organic Molecules on Silicon," *Phys. Rev. Lett* **98**, 066807 (2007).
402. P. Zhang, S. G. Louie, and M. L. Cohen, "Electron-Phonon Renormalization in Cuprate Superconductors," *Phys. Rev. Lett.* **98**, 067005 (2007). [Publisher's Note: *Phys. Rev. Lett.* **98**, 079901 (2007)]
403. S. Saito, S. G. Louie, and M. L. Cohen, "Site Selectivities of Alkali Ions in $\text{CsRb}_2\text{C}_{60}$ and $\text{Cs}_2\text{RbC}_{60}$ Superconductors," *Solid State Comm.* **142**, 186 (2007).
404. S. Saito, S. G. Louie, and M. L. Cohen, "Electronic Structure and Energetics of MgB_2 Nanotube," *J. Phys. Soc. Japan* **76**, 043707 (2007).
405. L. Yang, C. D. Spataru, S. G. Louie, and M. Y. Chou, "Enhanced Electron-hole Interaction and Optical Absorption in a Silicon Nanowire," *Phys. Rev. B* **75**, 201304 (2007).
406. J. Deslippe, C. D. Spataru, D. Prendergast, and S. G. Louie, "Bound Excitons in Metallic Single-walled Carbon Nanotubes," *Nano Lett.* **7**, 1626 (2007).
407. M.J. Comstock, N. Levy, A. Kirakosian, J. Cho, F. Lauterwasser, J.H. Harvey, D.A. Strubbe, J.M.J. Frechet, D. Trauner, S. G. Louie, and M. F. Crommie, "Reversible Photomechanical Switching of Individual Engineered Molecules at a Metallic Surface," *Phys. Rev. Lett.* **99**, 038301 (2007).
408. Y.Y. Wang, R. Yamachika, A. Wachowiak, M. Grobis, K. H. Khoo, D. H. Lee, S. G. Louie, and M. F. Crommie, "Novel Orientational Ordering and Reentrant Metallicity in KxC_{60} Monolayers for $3 \leq x \leq 5$," *Phys. Rev. Lett.* **99**, 086402 (2007).
409. C.-H. Park, F. Giustino, M. L. Cohen, and S. G. Louie, "Velocity Renormalization and Carrier Lifetime in Graphene from the Electron-Phonon Interaction," *Phys. Rev. Lett.* **99**, 086804 (2007).
410. H. J. Choi, M. L. Cohen, and S. G. Louie, "First-Principles Scattering-State Approach for Nonlinear Electrical Transport in Nanostructures," *Phys. Rev. B* **76**, 155420 (2007).
411. F. Giustino, M. L. Cohen, and S. G. Louie, "Electron-Phonon Interaction Using Wannier Functions," *Phys. Rev. B* **76**, 165108 (2007).
412. L. Yang, M. L. Cohen, and S. G. Louie, "Excitonic Effects in the Optical Spectra of Graphene Nanoribbons," *Nano Lett.* **7**, 3112 (2007).
413. S.Y. Quek, L. Venkataraman, H. J. Choi, S. G. Louie, M. S. Hybertsen, and J.B. Neaton, "Amine-Gold Linked Single-Molecule Circuits: Experiment and Theory," *Nano Lett.* **7**, 3477 (2007).
414. L. Yang, C.H. Park, Y.-W. Son, M. L. Cohen, and S. G. Louie, "Quasiparticle Energies and Band Gaps of Graphene Nanoribbons," *Phys. Rev. Lett.* **99**, 186801 (2007).
415. Y.-W. Son, M. L. Cohen, and S. G. Louie, "Electric Field Effects on Spin Transport in Defective Metallic Carbon Nanotubes," *Nano Letters* **7**, 3518 (2007).
416. R.B. Capaz, C. D. Spataru, S. Ismail-Beigi, and S. G. Louie, "Excitons in Carbon Nanotubes: Diameter and Chirality Trends," *Phys. Stat. Sol. (b)* **244**, 4016 (2007).

417. F. Wang, D.J. Cho, B. Kessler, J. Deslippe, P.J. Schuck, S. G. Louie, A. Zettl, T.F. Heinz, and Y. R. Shen, "Observation of Excitons in One-Dimensional Metallic Single-Walled Carbon Nanotubes," *Phys. Rev. Lett.* **99**, 227401 (2007).
418. L.Z. Kong, J. R. Chelikowsky, J.B. Neaton, and S. G. Louie, "Real-space Pseudopotential Calculations of Spin-dependent Electron Transport in Magnetic Molecular Junctions," *Phys. Rev. B* **76**, 235422 (2007).
419. B. Lee, L.-W. Wang, C. D. Spataru, and S. G. Louie, "Nonlocal Exchange Correlation in Screened-exchange Density Functional Methods," *Phys. Rev. B* **76**, 245114 (2007).
420. C. D. Spataru, S. Ismail-Beigi, R.B. Capaz, and S. G. Louie, "Quasiparticle and Excitonic Effects in the Optical Response of Nanotubes and Nanoribbons," in *Carbon Nanotubes: Advanced Topics in the Synthesis, Structure, Properties and Applications*, A. Jorio, M. S. Dresselhaus, G. Dresselhaus (eds.), Topics in Applied Physics **111** (Springer-Verlag, Heidelberg, Germany 2008), p. 195.
421. Y.Y. Wang, E. Kioupakis, X.H. Lu, D. Wegner, R. Yamachika, J. E. Dahl, R. M.K. Carlson, S. G. Louie, and M. F. Crommie, "Spatially Resolved Electronic and Vibronic Properties of Single Diamondoid Molecules," *Nature Mater.* **7**, 38 (2008).
422. J. Deslippe and S. G. Louie, "Excitons and Many-electron Effects in the Optical Response of Carbon Nanotubes and Other One-dimensional Nanostructures," *Proc. SPIE* **6892**, 68920U-1 (2008).
423. P. Zhang, S. Saito, S. G. Louie, and M. L. Cohen, "Theory of the Electronic Structure of Alternating MgB_2 and Graphene Layered Structures," *Phys. Rev. B* **77**, 052501 (2008).
424. C.-H. Park, L. Yang, Y.-W. Son, M. L. Cohen, and S. G. Louie, "Anisotropic Behaviours of Massless Dirac Fermions in Graphene under Periodic Potentials," *Nat. Phys.* **4**, 213 (2008).
425. C.-H. Park, F. Giustino, J.L. McChesney, A. Bostwick, T. Ohta, E. Rotenberg, M. L. Cohen, and S. G. Louie, "Van Hove Singularity and Apparent Anisotropy in the Electron-phonon Interaction in Graphene," *Phys. Rev. B* **77**, 113410 (2008).
426. K. H. Khoo, J.B. Neaton, H. J. Choi, and S. G. Louie, "Contact Dependence of the Conductance of H_2 Molecular Junctions from First Principles," *Phys. Rev. B* **77**, 115326 (2008).
427. Y.M. Byun, H. J. Choi, S. G. Louie, and M. L. Cohen, "Low-energy Structures of K Atoms in Expanded K_3C_{60} Monolayers: Ab Initio Pseudopotential Density-functional Calculations," *Phys. Rev. B* **77**, 115418 (2008).
428. E. Kioupakis, P. Zhang, M. L. Cohen, and S. G. Louie, "GW Quasiparticle Corrections to the LDA+U/GGA+U Electronic Structure of bcc Hydrogen," *Phys. Rev. B* **77**, 155114 (2008).
429. F. Giustino, M. L. Cohen, and S. G. Louie, "Small Phonon Contribution to the Photoemission Kink in the Copper Oxide Superconductors," *Nature* **452**, 975 (2008).
430. J. Noffsinger, F. Giustino, S. G. Louie, and M. L. Cohen, "First-principles Study of Superconductivity and Fermi-surface Nesting in Ultrahard Transition Metal Carbides," *Phys. Rev. B* **77**, 180507 (2008).
431. J.D. Sau, J.B. Neaton, H. J. Choi, S. G. Louie, and M. L. Cohen, "Electronic Energy Levels of Weakly Coupled Nanostructures: C_{60} -Metal Interfaces," *Phys. Rev. Lett.* **101**, 026804 (2008).
432. C.H. Park and S. G. Louie, "Energy Gaps and Stark Effect in Boron Nitride Nanoribbons," *Nano Lett.* **8**, 2200 (2008).

433. G. Kim, S. -H. Jhi, N. Park, S. G. Louie, and M. L. Cohen, "Optimization of Metal Dispersion in Doped Graphitic Materials for Hydrogen Storage," *Phys. Rev. B* **78**, 085408 (2008).
434. K. H. Khoo, J.B. Neaton, Y.W. Son, M. L. Cohen, and S. G. Louie, "Negative Differential Resistance in Carbon Atomic Wire-carbon Nanotube Junctions," *Nano Lett.* **8**, 2900 (2008).
435. C.-H. Park, Y.-W. Son, L. Yang, M. L. Cohen, and S. G. Louie, "Electron Beam Supercollimation in Graphene Superlattices," *Nano Lett.* **8**, 2920 (2008).
436. C.-H. Park, L. Yang, Y.-W. Son, M. L. Cohen, and S. G. Louie, "New Generation of Massless Dirac Fermions in Graphene under External Periodic Potentials," *Phys. Rev. Lett.* **101**, 126804 (2008).
437. L. Yang, M. L. Cohen, S. G. Louie, "Magnetic Edge-state Excitons in Zigzag Graphene Nanoribbons," *Phys. Rev. Lett.* **101**, 186401 (2008).
438. C.-H. Park, F. Giustino, M. L. Cohen, and S. G. Louie, "Electron-phonon Interactions in Graphene, Bilayer Graphene, and Graphite," *Nano Lett.* **8**, 4229 (2008). [Erratum: *Nano Lett.* **9**, 1731 (2009)]
439. J. B. Neaton, D. Prendergast, S. Whitlam, and S. G. Louie, "Understanding Nanoscale Systems at the Molecular Foundry," *SciDAC Review* **10**, 22 (2008).
440. C.-H. Park, F. Giustino, C. D. Spataru, M. L. Cohen, and S. G. Louie, "First-principles Study of Electron Linewidths in Graphene," *Phys. Rev. Lett.* **102**, 076803 (2009). [Erratum: *Phys. Rev. Lett.* **102**, 189904(E) (2009)]
441. H. J. Choi, S. G. Louie, and M. L. Cohen, "Anisotropic Eliashberg Theory for Superconductivity in Compressed and Doped MgB_2 ," *Phys. Rev. B* **79**, 094518 (2009).
442. C.O. Girit, J. C. Meyer, R. Erni, M.D. Rossell, C. Kisielowski, Li Yang, C.-H. Park, M. F. Crommie, M. L. Cohen, S. G. Louie, and A. Zettl, "Graphene at the Edge: Stability and Dynamics," *Science* **323**, 1705 (2009).
443. J. Noffsinger, F. Giustino, S. G. Louie, and M. L. Cohen, "Origin of Superconductivity in Boron-doped Silicon Carbide from First Principles," *Phys. Rev. B* **79**, 104511 (2009).
444. J. Deslippe, M. Dipoppa, D. Prendergast, M.V.O. Moutinho, R.B. Capaz, and S. G. Louie, "Electron-hole Interaction in Carbon Nanotubes: Novel Screening and Exciton Excitation Spectra," *Nano Lett.* **9**, 1330 (2009).
445. J. Noffsinger, S. G. Louie, F. Giustino, and M. L. Cohen, "Role of Fluorine in the Iron Pnictides: Phonon Softening and Effective Hole Doping," *Phys. Rev. Lett.* **102**, 147003 (2009).
446. C. D. Spataru, M. S. Hybertsen, S. G. Louie, and A.J. Millis, "GW Approach to Anderson Model out of Equilibrium: Coulomb Blockade and False Hysteresis in the I-V Characteristics," *Phys. Rev. B* **79**, 155110 (2009).
447. S.Y. Quek, M. Kamenetska, M. L. Steigerwald, H. J. Choi, S. G. Louie, M. S. Hybertsen, J.B. Neaton, and L. Venkataraman, "Mechanically Controlled Binary Conductance Switching of a Single-molecule Junction," *Nature Nanotechnol.* **4**, 230 (2009).
448. C.-H. Park and S. G. Louie, "Making Massless Dirac Fermions from a Patterned Two-dimensional Electron Gas," *Nano Lett.* **9**, 1793 (2009).
449. C.-H. Park, Y.-W. Son, L. Yang, M. L. Cohen, and S. G. Louie, "Landau Levels and Quantum Hall Effect in Graphene Superlattices," *Phys. Rev. Lett.* **103**, 046808 (2009).

450. H. J. Choi, S. G. Louie, and M. L. Cohen, "Prediction of Superconducting Properties of CaB_2 Using Anisotropic Eliashberg Theory," *Phys. Rev. B* **80**, 064503 (2009).
451. H. Lee, J. Ihm, M. L. Cohen, and S. G. Louie, "Calcium-decorated Carbon Nanotubes for High Capacity Hydrogen Storage: First-principles Calculations," *Phys. Rev. B* **80**, 115412 (2009).
452. L. Yang, J. Deslippe, C.-H. Park, M. L. Cohen, and S. G. Louie, "Excitonic Effects on the Optical Response of Graphene and Bilayer Graphene," *Phys. Rev. Lett.* **103**, 186802 (2009).
453. S.K. Choi, D.-H. Lee, S. G. Louie, and J. Clarke, "Localization of Metal-Induced Gap States at the Metal-Insulator Interface: Origin of Flux Noise in SQUIDs and Superconducting Qubits," *Phys. Rev. Lett.* **103**, 197001 (2009).
454. S.Y. Quek, H. J. Choi, S. G. Louie, and J.B. Neaton, "Length Dependence of Conductance in Aromatic Single-Molecule Junctions," *Nano Lett.* **9**, 3949 (2009).
455. C. Tao, J. Sun, X. Zhang, R. Yamachika, D. Wegner, Y. Bahri, G. Samsonidze, M. L. Cohen, S. G. Louie, T.D. Tilley, R.A. Segalman, and M. F. Crommie, "Spatial Resolution of a Type II Heterojunction in a Single Bipolar Molecule," *Nano Lett.* **9**, 3963 (2009).
456. C.-H. Park, F. Giustino, C. D. Spataru, M. L. Cohen, and S. G. Louie, "Angle-resolved Photoemission Spectra of Graphene from First-principles," *Nano Lett.* **9**, 4234 (2009).
457. D. Prendergast and S. G. Louie, "Bloch-state-based Interpolation: An Efficient Generalization of the Shirley Approach to Interpolating Electronic Structure," *Phys. Rev. B* **80**, 235126 (2009).
458. V.W. Brar, S. Wickenburg, M. Panlasigui, C.-H. Park, T.O. Wehling, Y. Zhang, R. Decker, C. Girit, A.V. Balatsky, S. G. Louie, A. Zettl, and M. F. Crommie, "Observation of Carrier-Density-Dependent Many-Body Effects in Graphene via Tunneling Spectroscopy," *Phys. Rev. Lett.* **104**, 036805 (2010).
459. T.-T. Tang, Y.B. Zhang, C.-H. Park, B.S. Geng, C. Girit, Z. Hao, M.C. Martin, A. Zettl, M. F. Crommie, S. G. Louie, Y. R. Shen, and F. Wang, "A Tunable Phonon-Exciton Fano System in Bilayer Graphene," *Nature Nanotechnol.* **5**, 32 (2010).
460. C.-H. Park and S. G. Louie, "Tunable Excitons in Biased Bilayer Graphene," *Nano Lett.* **10**, 426 (2010).
461. J. L. Janssen, J. Laflamme, M. Côté, S. G. Louie, and M. L. Cohen, "Electron-Phonon Coupling in C_{60} Using Hybrid Functionals," *Phys. Rev. B* **81**, 073106 (2010).
462. F. Giustino, M. L. Cohen, and S. G. Louie, "GW Method with the Self-Consistent Sternheimer Equation," *Phys. Rev. B* **81**, 115105 (2010).
463. B.D. Malone, S. G. Louie, and M. L. Cohen, "Electronic and Optical Properties of Body-Centered Tetragonal Si and Ge," *Phys. Rev. B* **81**, 115201 (2010).
464. H.K. Lee, J. Ihm, M. L. Cohen, and S. G. Louie, "Calcium-Decorated Graphene-Based Nanostructures for High-Capacity Hydrogen Storage," *Nano Lett.* **10**, 793 (2010).
465. M.J. Comstock, D.A. Strubbe, L. Berbil-Bautista, N. Levy, J. Cho, D. Poulsen, J. M. J. Frechet, S. G. Louie, and M. F. Crommie, "Determination of Photoswitching Dynamics through Chiral Mapping of Single Molecules Using a Scanning Tunneling Microscope," *Phys. Rev. Lett.* **104**, 178301 (2010).
466. O.V. Yazyev and S. G. Louie, "Topological Defects in Graphene: Dislocations and Grain Boundaries," *Phys. Rev. B* **81**, 195420 (2010).

467. L.Z. Tan, C.-H. Park, and S. G. Louie, "Graphene Dirac Fermions in One-dimensional Inhomogeneous Field Profiles: Transforming Magnetic to Electric Field," *Phys. Rev. B* **81**, 195426 (2010).
468. M. Kamenetska, S.Y. Quek, A.C. Whalley, M. L. Steigerwald, H. J. Choi, S. G. Louie, C. Nuckolls, M. S. Hybertsen, J.B. Neaton, and L. Venkataraman, "Conductance and Geometry of Pyridine-linked Single-molecule Junctions," *J. Am. Chem. Soc.* **132**, 6817 (2010).
469. F.D. Vila, D.A. Strubbe, Y. Takimoto, X. Andrade, A. Rubio, S. G. Louie, and J.J. Rehr, "Basis Set Effects on the Hyperpolarizability of CHCl_3 : Gaussian-type Orbitals, Numerical Basis Sets and Real-space Grids," *J. Chem. Phys.* **133**, 034111 (2010).
470. G.-S. Do, J. Kim, S. -H. Jhi, C.-H. Park, S. G. Louie, and M. L. Cohen, "Ab Initio Calculations of Pressure-induced Structural Phase Transitions of GeTe," *Phys. Rev. B* **82**, 054121 (2010).
471. B.-C. Shih, Y. Xue, P. Zhang, M. L. Cohen, and S. G. Louie, "Quasiparticle Band Gap of ZnO: High Accuracy from the Conventional G^0W^0 Approach," *Phys. Rev. Lett.* **105**, 146401 (2010).
472. O.V. Yazyev and S. G. Louie, "Electronic Transport in Polycrystalline Graphene," *Nat. Mater.* **9**, 806 (2010).
473. J. Noffsinger, F. Giustino, B.D. Malone, C.-H. Park, S. G. Louie, and M. L. Cohen, "EPW: A Program for Calculating the Electron-phonon Coupling Using Maximally Localized Wannier Functions," *Comput. Phys. Commun.* **181**, 2140 (2010).
474. H.K. Lee, M. L. Cohen, and S. G. Louie, "Selective Functionalization of Halogens on Zigzag Graphene Nanoribbons: A Route to the Separation of Zigzag Graphene Nanoribbons," *Appl. Phys. Letters* **97**, 233101 (2010).
475. F. Giustino, S. G. Louie, and M. L. Cohen, "Electron-phonon Renormalization of the Direct Band Gap of Diamond," *Phys. Rev. Lett.* **105**, 265501 (2010).
476. B.S. Geng, J. Horng, Y.B. Zhang, T.T. Tang, C.-H. Park, C. Girit, Z. Lao, M. Martin, A. Zettl, M. F. Crommie, S. G. Louie, and F. Wang, "Optical Spectroscopy of Bilayer Graphene," *Physica Stat. Solidi B* **247**, 2931 (2010).
477. E. Kioupakis, M. L. Tiago, and S. G. Louie, "Quasiparticle Electronic Structure of Bismuth Telluride in the GW Approximation," *Phys. Rev. B* **82**, 245203 (2010).
478. O.V. Yazyev, J. E. Moore, and S. G. Louie, "Spin Polarization and Transport of Surface States in the Topological Insulators Bi_2Se_3 and Bi_2Te_3 from First Principles," *Phys. Rev. Lett.* **105**, 266806 (2010).
479. V.W. Brar, R. Decker, H.-M. Solowan, Y. Wang, L. Maserati, K.T. Chan, H. Lee, C.O. Girit, A. Zettl, S. G. Louie, M. L. Cohen, and M. F. Crommie, "Gate-controlled Ionization and Screening of Cobalt Adatoms on a Graphene Surface," *Nature Physics* **7**, 43 (2011).
480. C.-H. Park, L.Z. Tan, and S. G. Louie, "Theory of the Electronic and Transport Properties of Graphene Under a Periodic Electric or Magnetic Field," *Physica E* **43**, 651 (2011).
481. S.Y. Quek, H. J. Choi, S. G. Louie, and J.B. Neaton, "Thermopower of Amine-Gold-linked Aromatic Molecular Junctions from First Principles," *ACS Nano* **5**, 551 (2011).
482. N. Alem, O.V. Yazyev, C. Kisielowski, P. Denes, U. Dahmen, P. Hartel, M. Haider, M. Bischoff, B. Jiang, S. G. Louie, and A. Zettl, "Probing the Out-of-Plane Distortion of Single Point Defects in Atomically Thin Hexagonal Boron Nitride at the Picometer Scale," *Phys. Rev. Lett.* **106**, 126102 (2011).

483. C.-F. Chen, C.-H. Park, B.W. Boudouris, J. Horng, B. Geng, C. Girit, A. Zettl, M. F. Crommie, R.A. Segalman, S. G. Louie, and F. Wang, "Controlling Inelastic Light Scattering Quantum Pathways in Graphene," *Nature* **471**, 617 (2011).
484. H. Oh, H. J. Choi, S. G. Louie, and M. L. Cohen, "Fermi Surfaces and Quantum Oscillations in the Underdoped High- T_c Superconductors $\text{YBa}_2\text{Cu}_3\text{O}_{6.5}$ and $\text{YBa}_2\text{Cu}_4\text{O}_8$," *Phys. Rev. B* **84**, 014518(2011).
485. D.A. Siegel, C.-H. Park, C. Hwang, J. Deslippe, A.V. Federov, S. G. Louie, and A. Lanzara, "Many-body Interactions in Quasi-freestanding Graphene," *Proc. Natl. Acad. Sci. U.S.A.* **108** 11365 (2011).
486. L.Z. Tan, C.-H. Park, and S. G. Louie, "New Dirac Fermions in Periodically Modulated Bilayer Graphene," *Nano Lett.* **11**, 2596 (2011).
487. C. Tao, L. Jiao, O.V. Yazyev, Y.-C. Chen, J. Feng, X. Zhang, R.B. Capaz, J.M. Tour, A. Zettl, S. G. Louie, H. Dai, and M. F. Crommie, "Spatially Resolving Edge States of Chiral Graphene Nanoribbons," *Nature Physics* **7**, 616 (2011).
488. H.C. Hsueh, G.Y. Guo, and S. G. Louie, "Excitonic Effects in the Optical Properties of an SiC Sheet and Nanotubes," *Phys. Rev. B* **84**, 85404 (2011).
489. G.P. Zhang, D.A. Strubbe, S. G. Louie, and T.F. George, "First-principles Prediction of Optical Second-order Harmonic Generation in the Endohedral N@C_{60} Compound," *Phys. Rev. A* **84**, 023837 (2011).
490. S. Blackburn, M. Cote, S. G. Louie, and M. L. Cohen, "Enhanced Electron-phonon Coupling Near the Lattice Instability of Superconducting $\text{NbC}_{1-x}\text{N}_x$ from Density-Functional Calculations," *Phys. Rev. B* **84**, 104506 (2011).
491. C. Hwang, C.-H. Park, D.A. Siegel, A.V. Fedorov, S. G. Louie, and A. Lanzara, "Direct Measurement of Quantum Phases in Graphene via Photoemission Spectroscopy," *Phys. Rev. B* **84**, 125422 (2011).
492. O.V. Yazyev, R.B. Capaz, S. G. Louie, "Theory of Magnetic Edge States in Chiral Graphene Nanoribbons," *Phys. Rev. B* **84**, 115406 (2011).
493. G. Samsonidze, M. Jain, J. Deslippe, M. L. Cohen, and S. G. Louie, "Simple Approximate Physical Orbitals for *GW* Quasiparticle Calculations," *Phys. Rev. Lett* **107**, 186404 (2011).
494. G. Samsonidze, M. L. Cohen, and S. G. Louie, "Compensation-doped Silicon for Photovoltaic Applications," *Phys. Rev. B* **84**, 195201 (2011).
495. M. Jain, J. R. Chelikowsky, and S. G. Louie, "Quasiparticle Excitations and Charge Transition Levels of Oxygen Vacancies in Hafnia," *Phys. Rev. Lett.* **107**, 216803 (2011).
496. M. Jain, J. R. Chelikowsky, and S. G. Louie, "Reliability of Hybrid Functionals in Predicting Band Gaps," *Phys. Rev. Lett.* **107**, 216806 (2011).
497. O.V. Yazyev, R.B. Capaz, and S. G. Louie, "One-dimensional Structural Irregularities in Graphene Chiral Edges and Grain Boundaries," *J. Physics: Conference Series* **302**, 012016 (2011).
498. C.-H. Park, F. Giustino, C. D. Spataru, M. L. Cohen, and S. G. Louie, "Inelastic Carrier Lifetime in Bilayer Graphene," *Appl. Phys. Lett.* **100**, 032106 (2012).
499. D. A. Strubbe, L. Lehtovaara, A. Rubio, M. A. L. Marques, and S. G. Louie, "Response Functions in TDDFT: Concepts and Implementation," in *Fundamentals of Time-Dependent Density Functional Theory* (LNP **837**); eds. M. A. L. Marques, N. T. Maitra, F. M. S. Nogueira, E. K. U. Gross, A. Rubio (Springer, Heidelberg, 2012).

500. O. V. Yazyev, E. Kioupakis, J. E. Moore, and S. G. Louie, "Quasiparticle Effects in the Bulk and Surface-state Bands of Bi₂Se₃ and Bi₂Te₃ Topological Insulators," *Phys. Rev. B* **85**, 161101 (2012).
501. J. Noffsinger, E. Kioupakis, C. G. Van de Walle, S. G. Louie, and M. L. Cohen, "Phonon-Assisted Optical Absorption in Silicon from First Principles," *Phys. Rev. Lett.* **108**, 167402 (2012).
502. K. H. Liu, J. Deslippe, F. J. Xiao, R. B. Capaz, X. P. Hong, S. Aloni, A. Zettl, W. L. Wang, X. D. Bai, S. G. Louie, E. G. Wang, and F. Wang, "An Atlas of Carbon Nanotube Optical Transitions," *Nat. Nanotechnol.* **7**, 325 (2012).
503. J. Deslippe, G. Samsonidze, D. A. Strubbe, M. Jain, M. L. Cohen, and S. G. Louie, "BerkeleyGW: A Massively Parallel Computer Package for the Calculation of the Quasiparticle and Optical Properties of Materials and Nanostructures," *Comput. Phys. Commun.* **183**, 1269 (2012).
504. K. Kim, S. Coh, L. Z. Tan, W. Regan, J. M. Yuk, E. Chatterjee, M. F. Crommie, M. L. Cohen, S. G. Louie, and A. Zettl, "Raman Spectroscopy Study of Rotated Double-layer Graphene: Misorientation-Angle Dependence of Electronic Structure," *Phys. Rev. Lett.* **108**, 246103 (2012).
505. M. Orlita, L. Z. Tan, M. Potemski, M. Sprinkle, C. Berger, W. A. de Heer, S. G. Louie, and G. Martinez, "Resonant Excitation of Graphene K-Phonon and Intra-Landau-Level Excitons in Magneto-Optical Spectroscopy," *Phys. Rev. Lett.* **108**, 247401 (2012).
506. X. Andrade, J. Alberdi-Rodriguez, D. A. Strubbe, M. J. T. Oliveira, F. Nogueira, A. Castro, J. Muguerza, A. Arruabarrena, S. G. Louie, A. Aspuru-Guzik, A. Rubio, and M. A. L. Marques, "Time-Dependent Density-Functional Theory in Massively Parallel Computer Architectures: the OCTOPUS Project," *J. Phys. Cond. Mat.* **24**, 233202 (2012).
507. J. Lischner, J. Deslippe, M. Jain, and S. G. Louie, "First-principles Calculations of Quasiparticle Excitations of Open-shell Condensed Matter Systems," *Phys. Rev. Lett.* **109**, 036406 (2012).
508. S. Choi, M. Jain, and S. G. Louie, "Mechanism for Optical Initialization of Spin in NV⁻ Center in Diamond," *Phys. Rev. B* **86**, 041202 (2012).
509. L. Song, L. Balicas, D. J. Mowbray, R. B. Capaz, K. Storr, L. Ci, D. Jariwala, S. Kurth, S. G. Louie, A. Rubio, and P. M. Ajayan, "Anomalous Insulator-Metal Transition in Boron Nitride-Graphene Hybrid Atomic Layers," *Phys. Rev. B* **86**, 075429 (2012).
510. C.-H. Park and S. G. Louie, "Spin Polarization of Photoelectrons from Topological Insulators," *Phys. Rev. Lett.* **109**, 097601 (2012).
511. N. Alem, Q. M. Ramasse, C. R. Seabourne, O. V. Yazyev, K. Erickson, M. C. Sarahan, C. Kisielowski, A. J. Scott, S. G. Louie, and A. Zettl, "Subangstrom Edge Relaxations Probed by Electron Microscopy in Hexagonal Boron Nitride," *Phys. Rev. Lett.* **109**, 205502 (2012).
512. S. Choi, J. Deslippe, R. B. Capaz, and S. G. Louie, "An Explicit Formula for Optical Oscillator Strength of Excitons in Semiconducting Single-Walled Carbon Nanotubes: Family Behavior," *Nano Lett.* **13**, 54 (2013).
513. X. W. Zhang, O. V. Yazyev, J. J. Feng, L. M. Xie, C. G. Tao, Y.-C. Chen, L. Y. Jiao, Z. Pedramrazi, A. Zettl, S. G. Louie, H. J. Dai, and M. F. Crommie, "Experimentally Engineering the Edge Termination of Graphene Nanoribbons," *ACS Nano* **7**, 198 (2013).
514. J. Lischner, D. Vigil-Fowler, and S. G. Louie, "Physical Origin of Satellites in Photoemission of Doped Graphene: An Ab Initio GW Plus Cumulant Study," *Phys. Rev. Lett.* **110**, 146801 (2013).

515. J. Deslippe, G. Samsonidze, M. Jain, M. L. Cohen, and S. G. Louie, "Coulomb-hole Summations and Energies for GW Calculations with Limited Number of Empty Orbitals: A Modified Static Remainder Approach," *Phys. Rev. B* **87**, 165124 (2013).
516. S. Coh, W. Gannett, A. Zettl, M. L. Cohen, and S. G. Louie, "Surface Atom Motion to Move Iron Nanocrystals through Constrictions in Carbon Nanotubes under the Action of an Electric Current," *Phys. Rev. Lett.* **110**, 185901 (2013).
517. C. Jozwiak, C.-H. Park, K. Gotlieb, C. Hwang, D.-H. Lee, S. G. Louie, J. D. Denlinger, C. R. Rotundu, R. J. Birgeneau, Z. Hussain, and A. Lanzara, "Photoelectron Spin-Flipping and Texture Manipulation in a Topological Insulator," *Nat. Phys.* **9**, 293 (2013).
518. Y. Wang, D. Wong, A. V. Shytov, V. W. Brar, S. Choi, Q. Wu, H.-Z. Tsai, W. Regan, A. Zettl, R. K. Kawakami, S. G. Louie, L. S. Levitov, and M. F. Crommie, "Observing Atomic Collapse Resonances in Artificial Nuclei on Graphene," *Science* **340**, 734 (2013).
519. S. Coh, S. G. Louie, and M. L. Cohen, "Theoretical Study of Solid Iron Nanocrystal Movement Inside a Carbon Nanotube," *Phys. Rev. B* **88**, 045424 (2013).
520. S. Coh, L. Z. Tan, S. G. Louie, and M. L. Cohen, "Theory of the Raman Spectrum of Rotated Double-layer Graphene," *Phys. Rev. B* **88**, 165431 (2013).
521. K. Kim, S. Coh, C. Kisielowski, M. F. Crommie, S. G. Louie, M. L. Cohen, and A. Zettl, "Atomically Perfect Torn Graphene Edges and Their Reversible Reconstruction," *Nat. Commun.* **4**, 2723 (2013).
522. D. Y. Qiu, F. H. da Jornada, and S. G. Louie, "Optical Spectrum of MoS₂: Many-body Effects and Diversity of Exciton States," *Phys. Rev. Lett.* **111**, 216805 (2013). [Erratum: *Phys. Rev. Lett.*, **115**, 119901 (2015)].
523. H.-C. Hsueh, G. Y. Guo, and S. G. Louie, "Electron and Optical Properties of Silicon Carbide Nanostructures," Chapter 7 in *Silicon-based Nanomaterials*, Springer Series in Materials Science **187**, 139 (eds. H. Li, J. Wu, Z.M. Wang) (2013).
524. Y. Sakai, G. D. Nguyen, R. B. Capaz, S. Coh, I. V. Pechenezhskiy, X. P. Hong, F. Wang, M. F. Crommie, S. Saito, S. G. Louie, and M. L. Cohen, "Intermolecular Interactions and Substrate Effects for an Adamantine Monolayer on a Au(111) Surface," *Phys. Rev. B* **88**, 235407 (2013).
525. T. Bazhiron, S. Coh, S. G. Louie, and M. L. Cohen, "Importance of Oxygen Octahedra Tilts for the Electron-Phonon Coupling in K-doped BaBiO₃," *Phys. Rev. B* **88**, 224509 (2013).
526. Q. Zhou, S. Coh, M. L. Cohen, S. G. Louie, and A. Zettl, "Imprint of Transition Metal d Orbitals on a Graphene Dirac Cone," *Phys. Rev. B* **88**, 235431 (2013).
527. S. Y. Wang, W. H. Wang, L. Z. Tan, X. G. Li, Z. L. Shi, G. W. Kuang, P. N. A. Liu, S. G. Louie, and N. A. Lin, "Tuning Two-Dimensional Band Structure of Cu(111) Surface-state Electrons that Interplay with Artificial Supramolecular Architectures," *Phys. Rev. B* **88**, 245430 (2013).
528. M. G. Menezes, R. B. Capaz, and S. G. Louie, "Ab Initio Quasiparticle Band Structure of ABA- and ABC-stacked Graphene Trilayers," *Phys. Rev. B* **89**, 035431 (2014).
529. A. Malashevich, M. Jain, and S. G. Louie, "First-principles DFT Plus GW Study of Oxygen Vacancies in Rutile TiO₂," *Phys. Rev. B* **89**, 075205 (2014).

530. J. Lischner, T. Bazhiron, A. H. MacDonald, M. L. Cohen, and S. G. Louie, "Effect of Spin Fluctuations on Quasiparticle Excitations: First-principles Theory and Application to Sodium and Lithium," *Phys. Rev. B* **89**, 081108 (2014).
531. J.-H. Chen, G. Autes, N. Alem, F. Gargiulo, A. Gautam, M. Linck, C. Kisielowski, O. V. Yazyev, S. G. Louie, and A. Zettl, "Controlled Growth of a Line Defect in Graphene and Implications for Gate-Tunable Valley Filtering," *Phys. Rev. B* **89**, 121407 (2014).
532. J. Lischner, D. Vigil-Fowler, and S. G. Louie, "Satellite Structures in the Spectral Functions of the Two-dimensional Electron Gas in Semiconductor Quantum Wells: A GW Plus Cumulant Study," *Phys. Rev. B* **89**, 125430 (2014).
533. A. Riss, S. Wickenburg, P. Gorman, L. Z. Tan, H.-Z. Tsai, D. G. de Oteyza, Y.-C. Chen, A. J. Bradley, M. M. Ugeda, G. Etkin, S. G. Louie, F. R. Fischer, and M. F. Crommie, "Local Electronic and Chemical Structure of Oligo-acetylene Derivatives Formed Through Radical Cyclizations at a Surface," *Nano Lett.* **14**, 2251 (2014).
534. K. F. Mak, F. H. da Jornada, K. L. He, J. Deslippe, N. Petrone, J. Hone, J. Shan, S. G. Louie, and T. F. Heinz, "Tuning Many-body Interactions in Graphene: The Effects of Doping on Excitons and Quasiparticle Lifetimes," *Phys. Rev. Lett.* **112**, 207401 (2014).
535. K. H. Liu, X. P. Hong, S. K. Choi, C. H. Jin, R. B. Capaz, J. Kim, W. L. Wang, X. D. Bai, S. G. Louie, E. G. Wang, and F. Wang, "Systematic Determination of Absolute Absorption Cross-Section of Individual Carbon Nanotubes," *Proc. Natl. Acad. Sci.* **111**, 7564 (2014).
536. A. Riss, S. Wickenburg, L. Z. Tan, H.-Z. Tsai, Y. Kim, J. Lu, A. J. Bradley, M. M. Ugeda, K. L. Meaker, K. Watanabe, T. Taniguchi, A. Zettl, F. R. Fischer, S. G. Louie, and M. F. Crommie, "Imaging and Tuning Molecular Levels at the Surface of a Gated Graphene Device", *ACS Nano* **8**, 5395 (2014).
537. M. Bernardi, D. Vigil-Fowler, J. Lischner, J. B. Neaton, and S. G. Louie, "Ab Initio Study of Hot Carriers in the First Picosecond after Sunlight Absorption in Silicon," *Phys. Rev. Lett.* **112**, 257402 (2014).
538. S. K. Choi, C.-H. Park, and S. G. Louie, "Electron Supercollimation in Graphene and Dirac Fermion Materials Using One-Dimensional Disorder Potentials," *Phys. Rev. Lett.* **113**, 026802 (2014).
539. G. Samsonidze, F.J. Ribeiro, M. L. Cohen, and S. G. Louie, "Quasiparticle and Optical Properties of Polythiophene-Derived Polymers," *Phys. Rev. B* **90**, 035123 (2014).
540. J. I. Mustafa, B. D. Malone, M. L. Cohen, and S. G. Louie, "Band Offsets in c-Si/Si-XII Heterojunctions," *Solid State Commun.* **191**, 6 (2014).
541. G. Samsonidze, M. L. Cohen, and S. G. Louie, "First-principles Study of Quasiparticle Energies of a Bipolar Molecule in a Scanning Tunneling Microscope Measurement," *Comput. Mater. Sci.* **91**, 187 (2014).
542. K. H. Liu, L. M. Zhang, T. Cao, C. H. Jin, D. Y. Qiu, Q. Zhou, A. Zettl, P. D. Yang, S. G. Louie, and F. Wang, "Evolution of Interlayer Coupling in Twisted MoS₂ Bilayers," *Nat. Commun.* **5**, 4966 (2014).
543. Z. L. Ye, T. Cao, K. O'Brien, H. Y. Zhu, X. B. Yin, Y. Wang, S. G. Louie, and X. Zhang, "Probing Excitonic Dark States in Single-layer Tungsten Disulphide," *Nature* **513**, 214 (2014).
544. J. Lischner, S. Sharifzadeh, J. Deslippe, J. B. Neaton, and S. G. Louie, "Effects of Self-Consistency and Plasmon-Pole Models on GW Calculations for Closed-Shell Molecules," *Phys. Rev. B* **90**, 115130 (2014).

545. M. Jain, J. Deslippe, G. Samsonidze, M. L. Cohen, J. R. Chelikowsky, and S. G. Louie, "Improved Quasiparticle Wave Functions and Mean Field for G0W0 Calculations: Initializations with the COHSEX Operator," *Phys. Rev. B* **90**, 115148 (2014).
546. M. Kapilashrami, G. Conti, I. Zegkinoglou, S. Nemsak, C. S. Conlon, T. Tomdahl, V. Fjallstrom, J. Lischner, S. G. Louie, R. J. Hamers, L. Zhang, J. H. Guo, C. S. Fadley, and F. J. Himpsel, "Boron Doped Diamond Films as Electron Donors in Photovoltaics: An X-ray Absorption and Hard X-ray Photoemission Study," *J. Appl. Phys.* **116**, 143702 (2014).
547. L. M. Zhang, K. H. Liu, A. B. Wong, J. Kim, X. P. Hong, C. Liu, T. Cao, S. G. Louie, F. Wang, and P. D. Yang, "Three-Dimensional Spirals of Atomic Layered MoS₂," *Nano Lett.* **14**, 6418 (2014).
548. S. Y. Wang, L. Z. Tan, W. H. Wang, S. G. Louie, and N. A. Lin, "Manipulation and Characterization of Aperiodical Graphene Structures Created in a Two-Dimensional Electron Gas," *Phys. Rev. Lett.* **113**, 196803 (2014).
549. M. M. Ugeda, A. J. Bradley, S. F. Shi, F. H. da Jornada, Y. Zhang, D. Y. Qiu, W. Ruan, S. K. Mo, Z. Hussain, Z. X. Shen, F. Wang, S. G. Louie, and M. F. Crommie, "Giant Bandgap Renormalization and Excitonic Effects in a Monolayer Transition Metal Dichalcogenide Semiconductor," *Nat. Mater.* **13**, 1091 (2014).
550. J. Lischner, T. Bazhiron, A. H. MacDonald, M. L. Cohen, and S. G. Louie, "First-principles Theory of Electron-spin Fluctuation Coupling and Superconducting Instabilities in Iron Selenide," *Phys. Rev. B* **91**, 020502 (2015).
551. Y-C, Chen, T. Cao, C. Chen, Z. Pedramrazi, D. Haberer, D. G. de Oteyza, F. R. Fischer, S. G. Louie, and M. F. Crommie, "Molecular Bandgap Engineering of Bottom-up Synthesized Graphene Nanoribbon Heterojunctions," *Nat. Nanotechnol.* **10**, 156 (2015).
552. F. Liu, L. Lin, D. Vigil-Fowler, J. Lischner, A. F. Kemper, S. Sharifzadeh, F. H. da Jornada, J. Deslippe, C. Yang, J. B. Neaton, and S. G. Louie, "Numerical Integration for Ab Initio Many-electron Self Energy Calculations within the GW Approximation," *J. Comput. Phys.* **286**, 1 (2015).
553. A. J. Bradley, M. M. Ugeda, F. H. da Jornada, D.Y. Qiu, W. Ruan, Y. Zhang, S. Wickenburg, A. Riss, J. Lu, S. K. Mo, Z. Hussain, Z.X. Shen, S. G. Louie, and M. F. Crommie, "Probing the Role of Interlayer Coupling and Coulomb Interactions on Electronic Structure in Few-Layer MoSe₂ Nanostructures," *Nano Lett.* **15**, 2594 (2015).
554. M. Bernardi, D. Vigil-Fowler, C. S. Ong, J. B. Neaton, and S. G. Louie, "Ab Initio Study of Hot Electrons in GaAs," *Proc. Natl. Acad. Sci.* **112**, 5291 (2015).
555. J. Lischner, G. K. Palsson, D. Vigil-Fowler, S. Nemsak, J. Avila, M. C. Asensio, C. S. Fadley, and S. G. Louie, "Satellite Band Structure in Silicon Caused by Electron-Plasmon Coupling," *Phys. Rev. B* **91**, 205113 (2015).
556. M. Bernardi, J. Mustafa, J. B. Neaton, and S. G. Louie, "Theory and Computation of Hot Carriers Generated by Surface Plasmon Polaritons in Noble Metals," *Nat. Commun.* **6**, 7044 (2015).
557. T. Cao, Z. L. Li, and S. G. Louie, "Tunable Magnetism and Half-Metallicity in Hole-Doped Monolayer GsSe," *Phys. Rev. Lett.* **114**, 236602 (2015).
558. L. Z. Tan, M. Orlita, M. Potemski, J. Palmer, C. Berger, W. A. de Heer, S. G. Louie, and G. Martinez, "SU(4) Symmetry Breaking Revealed by Magneto-optical Spectroscopy in Epitaxial Graphene," *Phys. Rev. B* **91**, 235122 (2015).

559. R. R. Cloke, T. Marangoni, G. D. Nguyen, T. Joshi, D. J. Rizzo, C. Bronner, T. Cao, S. G. Louie, M. F. Crommie, and F. R. Fischer, "Site-Specific Substitutional Boron Doping of Semiconducting Armchair Graphene Nanoribbons," *J. Am. Chem. Soc.* **137**, 8872 (2015).
560. S. Coh, M. L. Cohen, and S. G. Louie, "Large Electron-phonon Interactions from FeSe Phonons in a Monolayer," *New J. Phys.* **17**, 073027 (2015).
561. D. Y. Qiu, T. Cao, and S. G. Louie, "Nonanalyticity, Valley Quantum Phases, and Lightlike Exciton Dispersion in Monolayer Transition Metal Dichalcogenides: Theory and First-Principles Calculations," *Phys. Rev. Lett.* **115**, 176801 (2015).
562. J. I. Mustafa, S. Coh, M. L. Cohen, and S. G. Louie, "Automated Construction of Maximally Localized Wannier Functions: Optimized Projection Functions Method," *Phys. Rev. B* **92**, 165134 (2015).
563. M. J. van Setten, F. Carouso, S. Sharifzadeh, X. G. Ren, M. Scheffler, F. Liu, J. Lischner, L. Lin, J. R. Deslippe, S. G. Louie, C. Yang, F. Weigend, J. B. Neaton, F. Evers, and P. Rinke, "GW 100: Benchmarking G0W0 for molecular systems," *J. Chem. Theory Comput.* **11**, 5665 (2015).
564. G. R. Bhimanapati, Z. Lin, V. Meunier, Y. E. Jung, J. Cha, S. Das, D. Xiao, Y. Son, M. S. Strano, V. R. Cooper, L. B. Liang, S. G. Louie, E. Ringe, W. Zhou, S. S. Kim, R. R. Naik, B. G. Sumpter, H. Terrones, F. N. Xia, Y. L. Wang, J. Zhu, D. Akinwande, N. Alem, J. A. Schuller, R. E. Schaak, M. Terrones, and J. A. Robinson, "Recent Advances in Two-Dimensional Materials Beyond Graphene," *ACS Nano* **9**, 11509 (2015).
565. H. Z. Tai, A. A. Omrani, S. Coh, H. Oh, S. Wickenburg, Y. W. Son, D. Wong, A. Riss, H. S. Jung, G. D. Nguyen, G. F. Rodgers, A. S. Aikawa, T. Taniguchi, K. Watanabe, A. Zettl, S. G. Louie, J. Lu, M. L. Cohen, and M. F. Crommie, "Molecular Self-Assembly in a Poorly Screened Environment: F4TCNQ on Graphene/BN," *ACS Nano* **9**, 12168 (2015).
566. C. T. Chan, A. Fang, Z. Q. Zhang, and S. G. Louie, "Novel Transport Properties of Pseudospin-1 Photons." *SPIE Newsroom* (2015). DOI: 10.1117/2.1201512.006147
567. M. Y. Shao, F. H. da Jornada, C. Yang, J. Deslippe, and S. G. Louie, "Structure Preserving Parallel Algorithms for Solving the Bethe-Salpeter Eigenvalue Problem," *Linear Algebra Appl.* **488**, 148 (2016).
568. A. Fang, Z. Q. Zhang, S. G. Louie and C. T. Chan, "Klein Tunneling and Supercollimation of Pseudospin-1 Electromagnetic Waves," *Phys. Rev. B* **93**, 035422 (2016).
569. G. D. Nguyen, F. M. Tom, T. Cao, Z. Pedramrazi, C. Chen, D. J. Rizzo, T. Joshi, C. Bronner, Y. C. Chen, M. Favaro, S. G. Louie, F. R. Fischer, and M. F. Crommie, "Bottom-up Synthesis of N=13 Sulfur-Doped Graphene Nanoribbons," *J. Phys. Chem. C* **120**, 2684 (2016).
570. J. Lischner, S. Nemšák, G. Conti, A. Gloskovskii, G. K. Pálsson, C. M. Schneider, W. Drube, S. G. Louie, and C. Fadley, "Accurate Determination of the Valence Band Edge in Hard X-ray Photoemission Spectra Using GW Theory," *J. Appl. Phys.* **119**, 165703 (2016).
571. J. McClain, J. Lischner, T. Watson, D. A. Matthews, E. Ronca, S. G. Louie, T. C. Berkelbach, and G. K.-L. Chan, "Spectral Functions of the Uniform Electron Gas via Coupled-Cluster Theory and Comparison to the GW and Related Approximations," *Phys. Rev. B* **93**, 235139 (2016).
572. D. Y. Qiu, F. H. da Jornada, and S. G. Louie, "Screening and Many-body Effects in Two-Dimensional Crystals: Monolayer MoS₂," *Phys. Rev. B* **93**, 235435 (2016).
573. D. Vigil-Fowler, S. G. Louie, and J. Lischner, "Dispersion and Line Shape of Plasmon Satellites in One, Two, and Three dimensions," *Phys. Rev. B* **93**, 235446 (2016).

574. S. Coh, D.-H. Lee, S. G. Louie, and M. L. Cohen, "Proposal for a Bulk Material Based on a Monolayer FeSe on SrTiO₃ High-Temperature Superconductor," *Phys. Rev. B* **93**, 245138 (2016).
575. M. Y. Shao, L. Lin, C. Yang, F. Liu, F. H. Da Jornada, J. Deslippe, and S. G. Louie, "Low Rank Approximation in G_0W_0 Calculations," *Sci. China Math.* **59**, 1593 (2016).
576. L. Hung, F. H. da Jornada, J. Souto-Casares, J. R. Chelikowsky, S. G. Louie, and S. Ogut, "Excitation Spectra of Aromatic Molecules within a Real-Space GW-BSE Formalism: Role of Self-Consistency and Vertex Corrections," *Phys. Rev. B* **94**, 085125 (2016).
577. T. Cao, Z. L. Li, D. Y. Qiu, and S. G. Louie, "Gate Switchable Transport and Optical Anisotropy in 90° Twisted Bilayer Black Phosphorus," *Nano Lett.* **16**, 5542 (2016).
578. S. Coh, M. L. Cohen, and S. G. Louie, "Antiferromagnetism enables electron-phonon coupling in iron-based superconductors," *Phys. Rev. B* **94**, 104505 (2016).
579. J. I. Mustafa, S. Coh, M. L. Cohen, and S. G. Louie, "Automated construction of maximally localized Wannier functions for bands with nontrivial topology," *Phys. Rev. B* **94**, 125151 (2016).
580. J. I. Mustafa, M. Bernardi, J. B. Neaton, and S. G. Louie, "Ab initio electronic relaxation times and transport in noble metals," *Phys. Rev. B* **94**, 155105 (2016).
581. J. Li, Z. Tan, K. Zou, A. A. Stabile, D. J. Seiwel, K. Watanabe, T. Taniguchi, S. G. Louie, and J. Zhu, "Effective mass in bilayer graphene at low carrier densities: The role of potential disorder and electron-electron interaction," *Phys. Rev. B* **94**, 161406 (2016).
582. T. Pham, A. L. Gibb, Z. L. Li, S. M. Gilbert, C. Y. Song, S. G. Louie, and A. Zettl, "Formation and Dynamics of Electron-Irradiation-Induced Defects in Hexagonal Boron Nitride at Elevated Temperatures," *Nano Lett.* **16**, 7142 (2016).
583. H. R. Barzegar, A. Yan, S. Coh, E. Gracia-Espino, G. Dunn, T. Wagberg, S. G. Louie, M. L. Cohen, and A. Zettl, "Electrostatically Driven Nanoballoon Actuator," *Nano Lett.* **16**, 6787 (2016).
584. S. Wickenburg, J. Lu, J. Lischner, H. Z. Tsai, A. A. Omrani, A. Riss, C. Karrasch, A. Bradley, H. S. Jung, R. Khajeh, D. Wong, K. Watanabe, T. Taniguchi, A. Zettl, A. H. C. Neto, S. G. Louie, and M. F. Crommie, "Tuning charge and correlation effects for a single molecule on a graphene device," *Nat. Comm.* **7**, 13553 (2016).
585. G. Antonius, and S. G. Louie, "Temperature-Induced Topological Phase Transitions: Promoted versus Suppressed Nontrivial Topology," *Phys. Rev. Lett.* **24**, 246401 (2016).
586. J. Deslippe, F. da Jornada, D. Vigil-Fowler, T. Barnes, N. Wichmann, K. Raman, R. Sasanka, and S. G. Louie, "Optimizing excited-state electronic-structure codes for Intel Knights Landing: A case study on the BerkeleyGW software," in *International Conference on High Performance Computing*, pp. 402-414. Springer International Publishing, 2016.
587. L. Li, J. Kim, C. Jin, G. Ye, D. Y. Qiu, F. H. da Jornada, Z. Shi, L. Chen, Z. Zhang, F. Yang, K. Watanabe, T. Taniguchi, W. Ren, S. G. Louie, X. Chen, Y. Zhang, and F. Wang, "Direct Observation of Layer-Dependent Electronic Structure in Phosphorene," *Nat. Nanotechnol.* **12**, 21 (2017).
588. F. H. Jornada, D. Y. Qiu, and S. G. Louie, "Non-uniform sampling schemes of the Brillouin zone for many-electron perturbation-theory calculations in reduced dimensionality," *Phys. Rev. B* **95**, 035109 (2017).

589. T. Helm, F. Flicker, R. Kealhofer, P. J. W. Moll, I. M. Hayes, N. P. Breznay, Z. Li, S. G. Louie, Q. R. Zhang, L. Balicas, J. E. Moore, and J. G. Analytis, "Thermodynamic anomaly above the superconducting critical temperature in the quasi-one-dimensional superconductor Ta₄Pd₃Te₁₆," *Phys. Rev. B* **95**, 075121 (2017).
590. S. Coh, P. Y. Yu, Y. Aoki, S. Saito, S. G. Louie, and M. L. Cohen, "Alternative structure of TiO₂ with higher energy valence band edge," *Phys. Rev. B* **95**, 085422 (2017).
591. K. Hippalgaonkar, Y. Wang, Y. Ye, D. Y. Qiu, H. Zhu, Y. Wang, J. Moore, S. G. Louie, and X. Zhang, "High thermoelectric power factor in two-dimensional crystals of MoS₂," *Phys. Rev. B* **95**, 115407 (2017).
592. Z. Li, T. Cao, M. Wu, and S. G. Louie, "Generation of Anisotropic Massless Dirac Fermions and Asymmetric Klein Tunneling in Few-Layer Black Phosphorous Superlattices," *Nano Lett.* **17**, 2280 (2017).
593. A. Fang, Z. Q. Zhang, S. G. Louie, and C. T. Chan, "Anomalous Anderson localization behaviors in disordered pseudospin systems," *PNAS* 2017 **16**, 4087 (2017).
594. H. S. Sen, L. D. Xian, F. H. da Jornada, S. G. Louie, A. Rubio, "Ab initio Modelling of Plasmons in Metal-semiconductor Bilayer Transition-metal Dichalcogenide Heterostructures," *Israel Journal of Chem.* **57**, 540 (2017).
595. H. R. Barzegar, A. Yan, S. Coh, E. Gracia-Espino, C. Ojeda-Aristizabal, G. Dunn, M. L. Cohen, S. G. Louie, T. Wagberg, and A. Zettl, "Spontaneous twisting of a collapsed carbon nanotube," *Nano Res.* **10**, 1942 (2017).
596. C. Gong, L. Li, Z. Li, H. Ji, A. Stern, Y. Xia, T. Cao, W. Bao, C. Wang, Y. Wang, Z. Q. Qiu, R. J. Cava, S. G. Louie, J. Xia, and X. Zhang, "Discovery of intrinsic ferromagnetism in two-dimensional van der Waals crystals," *Nature* **546**, 265 (2017).
597. K. Gotlieb, Z. L. Li, C. Y. Lin, C. Jozwiak, J. H. Ryoo, C. H. Park, Z. Hussain, S. G. Louie, A. Lanzara, "Symmetry rules shaping spin-orbital textures in surface states," *Phys. Rev. B*, **95**, 245142 (2017).
598. D. Y. Qiu, F. H. da Jornada, S. G. Louie, "Environmental Screening Effects in 2D Materials: Renormalization of the Bandgap, Electronic Structure, and Optical Spectra, of Few-Layer Black Phosphorus," *Nano Lett.* **17**, 4706 (2017).
599. T. Cao, F. Zhao, S. G. Louie, "Topological Phases in Graphene Nanoribbons: Junction States, Spin Centers, and Quantum Spin Chains," *Phys. Rev. Lett.* **119**, 076401 (2017).
600. X. X. Zhang, T. Cao, Z. G. Lu, Y. C. Lin, F. Zhang, Y. Wang, Z. Q. Li, J. C. Hone, J. A. Robinson, D. Smirnov, S. G. Louie, T. F. Heinz, "Magnetic brightening and control of dark excitons in monolayer WSe₂," *Nat. Nanotechnol.* **12**, 9 (2017).
601. A. M. Yan, C. S. Ong, D. Y. Qiu, C. Ophus, J. Ciston, C. Merino, S. G. Louie, A. Zettl, "Dynamics of Symmetry-Breaking Stacking Boundaries in Bilayer MoS₂," *Journal of Phys. Chem. C*, **121**, 22559 (2017).
602. G. D. Nguyen, H. Z. Tsai, A. A. Omrani, T. Marangoni, M. Wu, D. J. Rizzo, G. F. Rodgers, R. R. Cloke, R. A. Durr, Y. Sakai, F. Liou, A. S. Aikawa, J. R. Chelikowsky, S. G. Louie, F. R. Fischer, M. F. Crommie, "Atomically precise graphene nanoribbon heterojunctions from a single molecular precursor," *Nature Nano.*, **12**, 1077 (2017).
603. L. Ju, L. Wang, T. Cao, T. Taniguchi, K. Watanabe, S. G. Louie, F. Rana, J.-W. Park, J. Hone, F. Wang, and P. L. McEuen, "Tunable excitons in bilayer graphene," *Science* **358**, 907 (2017).

Books

1. J. R. Chelikowsky and S. G. Louie, Editors: *Quantum Theory of Real Materials* (Kluwer Academic Press, Boston, 1996).
2. J. R. Chelikowsky, S. G. Louie, G. Martinez, and E. L. Shirley, Editors: *The Optical Properties of Materials*, MRS Symp. Proceed. Vol. **579** (Materials Research Society, Warrendale PA, 2000).
3. M. L. Cohen and S. G. Louie, vol. eds., *Conceptual Foundations of Materials: A Standard Model for Ground- and Excited-State Properties*; series eds. E. Burstein, M. L. Cohen, D.L. Mills, P.J. Stiles, *Contemporary Concepts of Condensed Matter Physics* (Elsevier, Amsterdam, 2006).
4. M. L. Cohen and S. G. Louie, *Fundamentals of Condensed Matter Physics* (Cambridge University Press, Cambridge, United Kingdom, 2016). ISBN: 978-0521513319

Reports

1. DD. P. Landau, F. F. Abraham, G. G. Batrouni, J. M. Carlson, J. R. Chelikowsky, D. D. Koelling, S. G. Louie, C. Mailhot, A. C. Switendick, P. R. Taylor, and A. R. Williams, National Research Council Report, *Computational and Theoretical Techniques for Materials Science* (National Academy Press, Washington, D.C., 1995).

Patents

1. M. L. Cohen, V. H. Crespi, S. G. Louie, and A. Zettl, "Metallic Carbon Materials," U.S. Patent #5,993,697 (11/30/1999).
2. V. H. Crespi, M. L. Cohen, S. G. Louie, and A. K. Zettl, "Nanotube Junctions," U.S. Patent #6,538,262 (03/25/2003).
3. V. H. Crespi, M. L. Cohen, S. G. Louie, and A. K. Zettl, "Nanotube Junctions," U.S. Patent #6,835,952 (12/28/2004).
4. J. P. Cumings, A. Zettl, S. G. Louie, and M. L. Cohen, "Telescoped Multiwall Nanotube and Manufacture Thereof," U.S. Patent #6,874,668 (04/05/2005).
5. C. R. Piskoti, A. K. Zettl, M. L. Cohen, M. Cote, J. C. Grossman, and S. G. Louie, "Carbon Based Thirty Six Atom Spheres," U.S. Patent #6,939,524 (09/06/2005).
6. J. P. Cumings, A. K. Zettl, S. G. Louie, and M. L. Cohen, "Telescoped Multiwall Nanotube and Manufacture thereof," U.S. Patent #7,238,425 B2 (07/03/2007).
7. C. Jozwiak, C.-H. Park, K. Gotlieb, S. G. Louie, Z. Hussain, and A. Lanzara, "Versatile spin-polarized electron source," U.S. Patent # 9,142,634 (09/22/2015).