Professor Michele Parrinello
Professor in Computational Sciences,
ETH, Zurich and Università della Svizzera Italiana USI, Lugano, Switzerland

THE UNIVERSITY OF CHICAGO

Pritzker School of Molecular Engineering

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Albert Einstein World Award of Science
Nomination of Prof. Michele Parrinello

Dear Sir/Madam,

With this letter, I would like to nominate Prof. Michele Parrinello for the Albert Einstein World Award of Science, and I would like to offer some comments on his outstanding scientific achievements.

Prof. Parrinello's development of ground-breaking methods for the simulation of molecules and materials has led to a new era in computer simulations, and to the creation of a new interdisciplinary field of atomistic simulations, encompassing chemistry, physics, materials and biological sciences. In essence *Parrinello is the main creator of a novel school of thought to understand and predict matter at the atomistic scale.*

Starting in the early 1980s, Parrinello and his various collaborators – Rahman, Car, Laio and others – have shown that simulations can be made realistic and thus predictive and falsifiable on the same footing as experiments and theories. As a result, the science of matter at the atomic scale can now walk on three legs rather than two (experiment and theory), with a predictive power believed to be impossible to reach a couple of decades ago.

The first scientific breakthrough of Michele Parrinello came with the realization of how to change the classical equations of motion of atoms and molecules to enable crystal structure transformations in computer simulations. His first application of this idea gave birth to what is now known as the Parrinello-Rahman method for the study of crystalline phase transitions. At the same time, Parrinello pioneered the use of Feynman's path integrals for the study of quantum effects, proposing a formulation,

which has now become the standard way of describing quantum effects in molecular simulations.

In 1985 Prof. Parrinello, together with Prof. R. Car, invented ab-initio molecular dynamics (MD), thus opening the new field of computer simulations from first principles, that is simulations based on the fundamental laws of quantum mechanics. The ab-initio MD method was first proposed in a paper in Physical Review Letters (cited more than 11700 times), and is now known as the Car-Parrinello method. The main idea was that of incorporating the complex electronic-based forces between atoms and molecules in molecular dynamics, thus unifying molecular dynamics and density functional theory (DFT) descriptions of atoms and molecules. Such unification brought about a double revolution in the microscopic understanding of condensed and molecular systems.

First, the unification of two methodologies belonging to originally distinct fields allowed scientists from different disciplines (chemistry, physics and materials science) to enter the realm of simulations of *dynamical* properties of matter based on quantum mechanical, first principles. In addition, the way this unification was carried out, from a technical standpoint, included a complete reformulation of the way DFT based calculations were performed, allowing one to tackle systems much bigger than ever studied before and thus qualitatively different. This opened the way to investigate brand new problems in chemistry and physics, completely out of reach before the advent of ab-initio MD. It is because of this ability to study new problems that ab-initio MD has become a truly novel investigation tool, complementary to experimental investigations as well as critical to the interpretation of increasingly complex experiments in chemistry and materials science. Calculations carried out with the Car-Parrinello method have not only complemented experiments, but also allowed one to explore details of condensed and molecular matter not directly accessible to experiment and stimulated new experimental investigations. Examples include simulations of surfaces and interfaces, complex chemical reactions under pressure and the study of realistic materials, including nanostructured materials, e.g. for use in the production of renewable energy sources.

In the year following the invention of the Car-Parrinello method, Michele Parrinello proposed another breakthrough in computer simulations, namely metadynamics, which permits the simulation and understanding of so-called rare events in dynamical simulations. These are important events that occur in nature too seldom to appear in the short time span of ordinary molecular dynamics simulations – often limited to nano or micro-seconds. Many groups all over the world now use refined forms of metadynamics to study and understand the behavior of complex molecules, including the behavior of proteins and other building blocks of life.

THE UNIVERSITY OF CHICAGO

In the last few years Parrinello, together with Omar Valsson, pushed the frontier of atomistic simulation yet further, by introducing **a** variational method that accomplishes the same results as metadynamics in a fraction of the computational time, and proposed a method to compute rates that opened the way to study completely new chemical processes.

In addition to inventing new methods and translating those in computer codes that revolutionized several fields, Parrinello himself applied the methods he invented to solve chemistry and physics problems, providing in-depth, original and predictive analysis of the systems studied. Noteworthy are the first simulation, carried out completely from first principles, of the melting of silicon, the simulation of solvated electrons, the very first simulations of liquid water and ions in water, which opened the field—completely unexplored before—of simulations of aqueous systems from first principles.

As expected given his ground breaking contributions to science, Michele Parrinello is a highly cited scientist, with a h-index of 143 and more than 101000 citations, he is a foreign member of the American Academy of Science and a Royal Society Fellow, among several other societies, and he is the recipients of numerous awards. He has trained many students and post-docs who, under his direction, have contributed to shape the fields he invented. I believe his accomplishments make him an ideal candidate to receive the prestigious Albert Einstein Award of Science.

Sincerely,

Giulia Galli

COLUMBIA UNIVERSITY

IN THE CITY OF NEW YORK

DEPARTMENT OF CHEMISTRY

December 2, 2019

Selection Committee
Einstein World Award of Sciences
World Cultural Council

To the Members of the Selection Committee:

It gives me great pleasure to enthusiastically support the nomination of Professor Michele Parrinello for the Einstein World Award of Science.

Prof. Parrinello has made so many major groundbreaking contributions to the methodology and application of computational science that it is difficult for me to do justice to them all and thus I will review only a few of his extremely important contributions here. Before his work, the simulation of condensed phases of matter largely ignored electronic processes. Molecular dynamics and Monte Carlo methods were readily applied to classical systems and although much was indeed learned from such simulations, many processes of importance in physics, chemistry and biology could not be properly simulated. These classical simulations were based on solving the classical equations of motion on assumed classical force fields, but in real systems the force field often changes when reactions take place, when external conditions of temperature and pressure change, or when systems undergo changes in phase. To account for such effects, it is necessary to include electronic quantum effects, and in some cases nuclear quantum effects. This was precisely what Michele Parrinello and Roberto Car did in their extraordinary groundbreaking paper 1985 paper (Car, R.; Parrinello, M, *Unified Approach for Molecular Dynamics and Density-Functional Theory*. Phys. Rev. Letts. 55 (22): 2471–2474 (1985), with more than 9,900 citations). Using an extended Lagrangian method they were able to formulate the problem by deriving a set of classical equations of motion for the nuclei and a set of classical equations for fictitious electronic degrees of freedom. This allowed them to simulate the dynamics of the nuclei on the ground state electronic energy surface consistent with the Born-Oppenheimer approximation. They were able to formulate this using density functional theory for the ground state of the system and were thus able to compute the *ab initio* force field on the fly. The method is now called CPMD (Car-Parrinello Molecular Dynamics) and it produced a revolution in the microscopic understanding of condensed matter in chemistry, physics, materials and the biological sciences.

Michele Parrinello (with Aneesur Rahman, deceased) (M Parrinello, A Rahman, *Polymorphic transitions in single crystals: A new molecular dynamics method*, J. App. Phys. 52, 7182-7190, (1981), with 4917 citations) were able to generalize the classical equations of motion of atoms and molecules to allow the periodic boundary conditions of molecular dynamics, (usually

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http://www.columbia.edu/cu/chemistry/groups/berne/

fixed in shape and size) to change shape and size in response to the motions of the atoms and molecules. Thus modification allowed them to simulate crystal structure transformations (phase transformations) by molecular dynamics. The first application of this idea gave birth to what is now known as the Parrinello-Rahman method for the simulation of crystalline phase transitions. This work opened the door to many studies of structural phase transitions and stress-strain relations in solids.

One of the major problems in the simulation complex systems is that the sampling is often non-ergodic on the relatively short time scales of the simulation. Enhanced sampling methods are thus needed to achieve thermodynamic accuracy. There are many enhanced sampling methods, some more efficient than others. Liao and Parrinello (Liao, A. Parrinello, M., Escaping free-energy minima, *Proc. Nat Acad. Sci.(USA)* 99 (20): 12562–12566 (2002)) devised an important and clever enhanced sampling method called Metadynamics (MTD, also abbreviated as METAD, or MetaD). This method is based on the choice of a few collective variables (functions of the position coordinates). One then runs full molecular dynamics in the full phase space of the system with the proviso that the probability of visiting a value of the chosen collective coordinate is reduced if the system has already visited that value. In this way one can more rapidly sample important basins on the potential energy surface and rapidly make transitions over energy barriers corresponding to the collective variables. In Metadynamics one corrects for the penalty and can thus determine the potential of mean force or free energy surface on which the collective variable moves. Of course the method's efficacy depends on the choice of collective variables. The method has been likened to the filling of the basins by virtual sand as time progresses. This clever method is currently a topic of considerable research. Parrinello has made important inroads into determining free energies of unbinding of ligands (drug molecules) from target protein receptors, an important problem for drug efficacy in cancer and other diseases. In a recent very exciting development Tiwary and Parrinello have shown how Metadynamics can be used to determine "off rates" of drug molecules from protein receptors (P. Tiwary and M. Parrinello, *From Metadynamics to Dynamics*, Phys. Rev. Lett. 111 230602 (2013)) These rates are very slow on a molecular time scale ranging from seconds to minutes and can thus not be determined by the usual methods even using state of the art computers like computers like ANTON which can simulate time scales up to milliseconds. In designing anticancer drugs medicinal chemists aim for ligands that stay bound for long times and these new methods will aid them in this quest by sorting candidates according to both binding affinity and slow off rates. Many groups all over the world now use refined forms of metadynamics to study and understand the behavior of complex molecules, including the behavior of proteins and other building blocks of life.

These are just a few of the many methods Parrinello and coworkers have invented. He has applied these methods to solve many important problems in chemistry, physics, material science, and biology, providing in-depth, original and predictive analyses of condensed matter systems. He provided the first simulations, carried out completely from first principles, of the melting of silicon, the simulation of solvated electrons, the very first simulations of liquid water and ions in water, which opened the field—completely unexplored before—of simulations of aqueous systems from first principles.

Michele Parrinello is a highly cited scientist, with an h-index of 124 and more than 70,800 citations, a foreign member of the National Academy of Science (USA) and a Fellow of the Royal Society (UK). He is the recipient of numerous awards, as listed in the nomination form. He has

had a major impact on condensed matter sciences and computational biology. Great inventiveness, imagination, and a deep understanding of molecular systems characterize his work. Although others have made striking contributions to this field, I believe Michele Parrinello's scientific accomplishments make him an outstanding candidate to receive the prestigious Einstein World Award in Science.

Sincerely yours,

Bruce J. Berne
Higgins Professor of Chemistry,
And Professor of Chemical Engineering
Columbia University

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Gregory A. Voth, Ph.D.
Haig P. Papazian Distinguished Service Professor
Department of Chemistry
James Franck Institute
Institute for Biophysical Dynamics
Senior Fellow of the Computation Institute

November 30, 2019

Selection Committee
Einstein World Award of Science
World Cultural Council

To the Members of the Selection Committee:

It is my great honor to support the nomination Professor Michele Parrinello of ETH Zurich/USI Lugano for the 2020 Einstein World Award of Science. Parrinello has been one of the most influential members of the chemistry and physical science community for nearly fifty years. He is a true pioneer in the field of theoretical and computational chemistry, as I will describe in this letter.

It is important to first recognize that there has been a tremendous growth of theory and computation within the field of chemistry and the related sciences due to a constant stream of innovative theoretical ideas combined with phenomenal increases in computer power. In my opinion and that of many others, no scientist is more responsible than Michele Parrinello for this remarkable evolution of the field theoretical and computational chemistry. He has developed *both* ground-breaking theoretical and computational methods, creatively combined them, and then gone on to solve numerous important problems in the chemical sciences. Parrinello has arguably provided much of the unifying basis for rigorous statistical mechanics within computer simulation and, even more importantly, for statistical mechanics with quantum mechanics, also within the computer simulation context.

The main focus of Parrinello's research has been to improve upon the molecular dynamics (MD) simulation methodology, greatly extend its scope, and apply it in innovative and insightful ways to a variety of important systems. As the power of computers has increased, so has the popularity of atomistic-based simulations increased, and there is no area of chemistry, biology, materials science, and many other fields of science in which simulations are not applied. Up front, the vast impact of Parrinello might be easily judged from his huge number of citations and from the fact that hardly any paper that uses atomistic simulations, in particular those based on MD, fails to cite one or more of his works - and if they do not, one feels that they should have. Parrinello's contributions have been historical and defining contributions in our field as I will outline below. In order to do this, I will follow the scientific evolution of this great scientist as a function of time, and I will attempt to highlight (only some of) the landmark contributions he has made to theoretical and computational chemistry along the way.

A formative moment in Parrinello's career was his sabbatical at Argonne National Laboratory, lasting almost two years, where he was introduced by Aneesur Rahman to atomistic MD simulation. At that time, atomistic MD was a discipline confined to a small group of specialists that required access to large computers and was rather limited in scope. During his time at ANL, Parrinello developed the so-called Parrinello-Rahman method. This method, which creatively utilized the idea of an extended simulation phase space (or extended Lagrangian), allowed

crystal to crystal phase transitions to be simulated under the condition of constant external stress. Now many years after its publication, this work still receives well in excess of 600 citations a year. In order to appreciate the relevance of this work one should go back in time to when it was developed. In those days, atomistic MD calculations were performed under conditions of constant volume. Parrinello and Rahman realized that by making the molecular dynamics cell vary in size and shape via the extended phase space approach, a whole new class of phenomena could be simulated. In a fashion that is typical of the way Parrinello conducts his research, he not only developed the method, but he also applied it to interesting systems of practical interest. In this case he studied the transition to the superionic state in AgI, a system that is still of interest to this day. This transition is accompanied by a crystal phase transition for which the Parrinello-Rahman method facilitated the simulation study. *This particular work is an example of where Parrinello unified computer simulation with rigorous statistical mechanics in order study key phenomena.*

During the same period, Parrinello studied the properties of an electron dissolved in a molten salt – arguably first application of the Feynman path integral formulation of quantum statistical physics to a realistic system. This was pioneering work also in another respect, in that it was suggested that the Feynman imaginary time action functional could be sampled by MD (path integral MD), an approach that is now widely used, even in quantum chromodynamics and which is at the heart of methods for simulating quantum dynamics such as centroid MD or ring polymer MD.

Upon Parrinello's return to Trieste, where he had a permanent position, he was concerned by the ability of current empirical force fields to describe the properties of materials. He first developed a new class of potential, the "glue" model, aimed at describing metallic binding. These model potentials are very similar to the popular embedded atoms model and the model was published about at the same time. Importantly, however, his quest for better potentials culminated in the development of *ab-initio* molecular dynamics (AIMD), or the Car-Parrinello method as it is also commonly called. This method combines a density functional theory calculation of the interatomic forces with MD in an elegant way involving, again, an extended Lagrangian approach. At the time such a feat was deemed not possible and, without exaggeration, it has revolutionized both the field of electronic structure calculations and that of molecular simulation. *The impact of this work has been enormous, bringing together communities that were separated, hence unifying statistical mechanics with quantum mechanics within the simulation field.*

Once this remarkable breakthrough was achieved, a flurry of applications followed. It is impossible here to review them all, so I will mention just two important applications in which the abilities of the Car-Parrinello method were exploited. In one of the first applications the melting of silicon was studied and it was shown that the AIMD method was able to describe the change in bonding from semi-conducting to metallic upon melting, a process that is very hard to simulate using standard potentials. Another pioneering area of focus was on the properties of water and water solutions, and in particular the study of the two water ions H^+ and OH^-. Both of these AIMD studies where landmarks, in no small way facilitated by this remarkable

breakthrough in computer simulation methodology.

Parrinello's interest in AIMD has continued over the years, leading to improvements of the method and the instruments of its analysis. A constant preoccupation has been to make contact with experiments, and he has therefore devised methods to extract from AIMD measurable quantities like infrared or Raman spectra, and NMR chemical shifts. Other applications of AIMD cover a wide variety of fields, from catalysts of industrial interest, to enzymes, to DNA, and to minerals and crystals under pressure.

In performing these AIMD and other MD simulations, Parrinello was always frustrated by their high computational cost, which limited the time scale over which the evolution of the system could be followed. To him and to others, this appeared as one of the most severe limits of MD methodology, a hurdle that cannot be overcome by sheer computational power. For this reason, Parrinello introduced and developed metadynamics (MetaD), an enhanced sampling method that has been a huge breakthrough for both academia and industry. (This method has also been complemented very recently by a variational approach that may have even greater efficacy and impact.) In working with my own graduate student, James Dama, Michele was able to prove that the MetaD approach is indeed exact (published in PRL, 2014). MetaD has additionally been shown to allow for the calculation of the *dynamical* rates of rare events such has the residence time of a drug in the binding site of a protein.

In conclusion, the MD simulation methods and their exemplary application by Michele Parrinello have defined and pushed forward the frontiers of theoretical and computational chemistry, allowing for a large number of problems of practical interest to be solved. His solutions are simple and elegant and the analysis of the simulation results innovative and insightful. He has also mentored a very large number of students and postdocs who now occupy important positions across the world in both academia and industry. He has also made the fruits of his research accessible to a vast community of researchers. Some of the most widely used codes for AIMD simulation (CPMD and CP2K) originated in his group and are accessible free of charge to academics, as is the metadynamics plug-in PLUMED that has been interfaced with many MD simulation codes.

Michele Parrinello is thus a truly great theoretical and computational chemist – and one who has revolutionized our field. He is clearly deserving of the Einstein World Award of Science.

Sincerely yours,

Gregory A. Voth, Ph.D.
Haig P. Papazian Distinguished Service Professor

Resume of Prof. Michele Parrinello

The scientific activity of Michele Parrinello spans more than four decades and has had a vast impact in many areas of science. A topical moment in his career was his sabbatical at Argonne National Laboratory, lasting almost two years, where he was introduced by Aneesur Rahman to atomistic molecular dynamics simulations. At that time atomistic simulation was a discipline confined to a small group of specialists that required access to large computers and was rather limited in scope.
The leitmotif of his investigations has been to improve the methodology first, then extend its scope by inventing new methods, and apply them in innovative and insightful ways to a variety of important systems. As the power of computers has increased, so has the popularity of atomic-based simulations increased also and there is no area of physical chemistry, biology, and very many other fields of science in which simulations are not applied.

The role and impact of Michele Parrinello can be judged from the vast number of citations and from the fact that hardly any paper that uses atomistic simulations, in particular those based on molecular dynamics, fails to cite one or more of his works - and if they do not, one feels that they should have.

For the sake of brevity, we shall not discuss the work he performed before meeting Rahman, although some little gems could also be found there, but move directly to highlighting the contributions he has made since he met Rahman.
During his time in Chicago he developed the so-called Parrinello-Rahman method. This method allows crystal to crystal phase transition under the condition of constant external stress. So many years after its publication, this work still received well in excess of 600 citations in the last year alone. In order to appreciate the relevance of this work we should go back to the time when it was developed. In those days atomistic calculations were performed under conditions of constant volume. Parrinello and Rahman realized that by making the molecular dynamics cell vary in size and shape, a whole new class of phenomena could be simulated. In a fashion that is typical of the way Parrinello conducts his research, he not only developed the method but he applied it to interesting systems of practical interest. In this case he studied the transition to the superionic state in AgI, a system that is still of interest to this day. This transition is accompanied by a crystal phase transition of which the Parrinello-Rahman method permitted the study.

In the same period he studied the properties of an electron dissolved in a molten salt - possibly the first application of the Feynman path integral formulation of quantum statistical physics to a realistic system. This was a pioneering work also in another respect, in that there it is suggested that the Feynman action could be sampled by molecular dynamics, an approach that is now used in quantum cromo-dynamics and which is at the heart of methods for simulating quantum dynamics such as centroid dynamics or path integral molecular dynamics.

Upon his return to Trieste, where he had a permanent position, he started occupying himself with the ability of current force fields to describe well the properties of

materials. For this reason he developed a new class of potential, the “glue” model aimed at describing metallic binding. These model potentials are very similar to the popular embedded atoms model and the model was published about at the same time. This search for better potentials culminated in the development of *ab-initio* molecular dynamics, or the Car-Parrinello method as it is also commonly called. This method combines density functional theory calculation of the interatomic forces with molecular dynamics in a rather elegant way. At the time such a feat was deemed not to be possible and it revolutionized both the field of electronic structure calculations and that of molecular dynamics. The impact and resonance of this work were enormous, bringing together communities that were separated.

Once this Pandora’s box was opened, a flurry of applications followed. It is difficult here to review them all, so we will mention just two remarkable applications in which the abilities of the Car-Parrinello method were exploited. In one of the first applications, the melting of silicon was studied and it was shown that the ab-initio method was able to describe the change in bonding from semi-conducting to metallic upon melting, a process that is hard to simulate using standard potentials. Another area of interest was the properties of water and water solutions and in particular the study of the two water ions H^+ and OH^-.
His interest in waters has continued over the years, improving methods and instrument of analysis. A constant preoccupation has been to make contact with the experiments, and he has therefore devised methods to extract from *ab-initio* molecular dynamics runs measurable quantities like infra-red or Raman spectra, or NMR chemical shifts. Other applications cover a wide variety of fields, from catalysts of industrial interest, to enzymes, to DNA, and to minerals and crystals under pressure.

In performing these simulations he was always frustrated by their high computational cost, which limited the time scale over which the evolution of the system could be followed. To him this looked like one of the most severe limits of molecular dynamics methods, a hurdle that could not be cleared by sheer computational power. For this reason, he introduced and developed metadynamics, an enhanced sampling method that has become very popular in both academe and industry. This method has been complemented very recently by a variational approach that promises to have even greater efficacy and impact. The method has proven to be exact and also allows the calculation of rates for rare events such has the residence time of a drug in the binding site of a protein, a parameter of critical relevance in the computer design of a drug.

In conclusion, the methods and the exemplary applications developed by Parrinello have pushed forward the frontiers of simulations, allowing a large number of problems of practical interest to be resolved. His solutions are simple and elegant and the analysis of the simulation results innovative and insightful. He has had a very large number of students and enthusiastic followers who now occupy important positions across the world in both academe and industry. He has made the fruits of his research accessible to the vast community of researchers. Some of the most used codes for *ab-initio* molecular dynamics simulation (CPMD and CP2K) originated in his group and are accessible free of charge to academics, as is the metadynamics plug-in PLUMED that can be interfaced with many simulation codes.

Michele Parrinello

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Tel. + 41-58-6664801, e-mail: parrinello@phys.chem.ethz.ch

Personal information

Date and Place of birth: 7 September 1945, Messina, Italy
Residence: Lugano, Switzerland

Education

Italian *Laurea* in physics, University of Bologna, 1968
PhD supervisor: Prof. Dr. Bruno Ferretti, Bologna
Postdoctoral supervisor: Prof. Dr. Mario Tosi

Professional experience

Professor in Computational Sciences, ETH, Zurich and Università della Svizzera Italiana USI, Lugano, Switzerland, 2001-present
Director, Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany, 1994-2001
Manager, IBM Research Laboratory, Zurich, Switzerland, 1991-1994
Research Staff Member, IBM Research Laboratory, Zurich, Switzerland, 1989-1991
Summer Visitor, IBM Research Laboratory, Zurich, Switzerland, 1987
Full Professor, International School for Advanced Studies (SISSA), Trieste, Italy, 1986-1989
Summer Visitor, University of Minnesota, Minneapolis, USA, 1986
Summer Visitor, IBM Research Laboratory, Yorktown, USA, 1985
Associate Professor, University of Trieste, Italy, 1982-1986
Visiting Scientist, Argonne National Laboratory, Chicago, USA, 1980-1981
Lecturer, University of Trieste, Italy, 1976-1982
Visiting Scientist, Imperial College, London, UK, 1975-1976
Lecturer, University of Messina, Italy, 1972-1977
Borsista del Consiglio Nazionale delle Ricerche, University of Messina, Italy, 1970-1971

Awards and Distinctions

Hewlett-Packard Europhysics Prize (with R. Car), European Physical Society (1990)
Boys-Rahman Prize, Royal Society of Chemistry, UK (1994)
Rahman Prize (with R. Car), American Physical Society (1995)
Award in Theoretical Chemistry, American Chemical Society (2001)
Schroedinger Medal of the World Association of Theoretically Oriented Chemists (2005)
Triennial Somaini Physics Prize, Italian Physical Society (2006)
Gutenberg Lecture Award, University of Mainz, Germany (2008)
FOMMS Medal Award, University of Michigan, USA (2009)
Sidney Fernbach Award (with R. Car), IEEE Computer Society, USA (2009)
Dirac Medal (with R. Car), ICTP Trieste, Italy (2009)
Berni J. Alder CECAM Prize (with R. Car), CECAM, Switzerland (2010)
Marcel Benoist Prize, Marcel Benoist Stiftung, Federal Dept. of Home Affairs, Switzerland (2011)
Enrico Fermi Prize, Italian Physical Society, Italy (2012)
Hirschfelder Prize, University of Wisconsin-Madison, USA (2012)
Grande Ufficiale della Repubblica Italiana (2012)
The Dreyfus Prize in Theoretical and Computational Chemistry, The Camille and Henry Dreyfus Foundation, New York, USA (2017)
ISQBP President's Award, The International Society of Quantum Biology and Pharmacology, Barcelona, Spain (2018)
Ertl Lecture Award, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, German

Honorary degrees

Honorary Doctorate in Chemistry, University of Messina, Italy (2003)
Honorary Doctorate in Materials Science and Technology, University of Rome 2, Italy (2005)
Honorary Doctorate in Materials Science, University of Cagliari, Sardinia, Italy (2006)
Honorary Doctorate in Industrial Chemistry, University of Como, Italy (2007)
Honorary Doctorate in Physics and Chemistry of Biological Systems, Scuola Internazionale Superiore di Studi Avanzati, SISSA, Trieste, Italy (2008)
Honorary Doctorate in Science, King's College, London, UK (2011)
Honorary Doctorate in Science, University of St. Andrews, Scotland (2012)
Honorary Doctorate in Science, Università degli Studi di Messina, Italy (2015)

Honorary academic appointments

Honorarprofessor, University of Stuttgart, Germany (1995)
Honorary Fellow, Sidney Sussex College, Cambridge, UK (2005)
Distinguished Visiting Professor, University of California, Santa Barbara, USA (2006/2007)
Adjunct Professor, Università della Svizzera Italiana, Lugano, Switzerland (2006)
Honorary Fellow, St. Catherine's College, Oxford, UK (2007)
Honorary Professor, East China University of Science and Technology, Shanghai, China (2008)

Named lectures

Eli Burstein Lecturer in Materials Science, University of Pennsylvania, USA (1993)
Gilbert Newton Lewis Lecturer, University of California, Berkeley, USA (2001)
DuPont-Marshall Lecturer, University of Pennsylvania, Philadelphia, USA (2001)
Lise Meitner Lecturer, Lise Meitner-Minerva Center for Computational Quantum Chemistry, Jerusalem, Israel (2001/2002)
Celsius Lecturer, Uppsala University, Sweden (2002)
Falk-Plaut Lecturer, Columbia University, New York, USA (2002)
Jean Perrin Lecturer, Chemical Physics Division, Physical and Chemical Societies, France (2003)
Linnett Visiting Professor, Cambridge University, UK (2005)
Cyril Hinshelwood Lecturer, Oxford University, UK (2006/2007)
Greg Watson Lecturer, Rutherford Appleton Laboratory, Didcot, UK (2007)
Charles A. Coulson Lecturer, University of Georgia, Athens, USA (2008)
Richard M. Noyes Lecturer, University of Oregon, Eugene, USA (2009)
Almlöf-Gropen Lecturer, Centre for Theoretical and Computational Chemistry, Norway (2010)
Arthur William Scott Lecturer, Cavendish Laboratory, Cambridge University, UK (2012)
Mulliken Lecturer, University of Chicago, Chicago, USA (2012)
Aneesur Rahman Lecturer, Argonne National Laboratory, Argonne, USA (2012)
Charlemagne Distinguished Lecture, RWTH Aachen University, Aachen, Germany (2013)
Pitzer Lecture, Ohio State University, Columbus, USA (2013)
Faraday Discussion, Royal Society, Cambridge, UK (2016)
Colloquium Ehrenfestii, Leiden, the Netherlands (2016)

Academy and learned society memberships

Fellow, American Physical Society (1991)
Socio corrispondente, Accademia dei Pericolanti, Italy (1992)
Member, International Academy of Quantum Molecular Science (1995)
Honorary Member of the Materials Research Society of India (1999)
Member, Berlin-Brandenburgische Akademie der Wissenschaften, Germany (2000)
External Scientific Member, Max Planck Society, Germany (2001-2012)
Foreign Member of the Royal Society, UK (2004)
Member, European Academy of Sciences (2004)
Fellow, World Association of Theoretically Oriented Chemists (WATOC) (2005)
Socio corrispondente, Accademia Nazionale dei Lincei, Roma, Italy (2005)

Foreign Member, *Istituto Lombardo, Accademia di Scienze e Lettere*, Milan, Italy (2007)
Foreign Member, The National Academy of Sciences, USA (2010)
Foreign Member, The American Academy of Arts and Sciences, USA (2012)
Socio nazionale, Accademia Nazionale dei Lincei, Rome, Italy (2014)

Society memberships

American Physical Society, American Chemical Society, Institute of Physics, Swiss Chemical Society, Italian Physical Society,

Research interests

Computer simulations and modelling of condensed matter, chemical and biophysical systems:
Ab-initio molecular dynamics, Metadynamics, Simulation of rare events, Structural and chemical transformations in solids under the effect of pressure, Nucleation, Chemical reactions in condensed phases, Protein-protein interaction

Publications

Over 600 research papers, review articles and edited books. His work has been cited more than 50'000 times, which makes him one of the most cited authors in physics and chemistry in the world. In particular, the first paper with Roberto Car is *Physical Review Letters*' 5th most cited of all time. His h-index is 121.

Current and past advisory activities

Microsoft Science Advisory Board, Redmond, USA
International Centre for Science and High Technology (ICS), Trieste, Italy
International School for Advanced Studies, (SISSA), Trieste, Italy
Scientific Council of the Fondazione Bruno Kessler, Trento, Italy
Scientific Council of the Fondazione Silvio Tronchetti Provera, Milan, Italy
Scientific Council of the Department of Materials and Devices, National Research Council, (INR), Rome, Italy
Board of Centro E. Fermi, Rome, Italy
Scientific Council of CINECA, Casalecchio di Reno (Bologna), Italy
Scientific Council of the National Institute of Chemistry, Ljubljana, Slovenija
Advisory Council of RIKEN Advanced Institute for Computational Science (AICS), Kobe, Japan

Editorial activities

Has been or is a member of the editorial advisory board of:
Chemical Physics, Chemical Physics Letters, ChemPhysChem, Computational Materials Science, Computing in Science and Engineering, Journal of Computer-Aided Materials Design, Journal of Physics, Science, Theoretical Chemistry Accounts

Refereeing

Research proposals from Austria, Canada, Germany, Italy, Netherlands, Switzerland, United Kingdom, United States.
Scientific articles from *Europhysics Letters, Journal of Chemical Physics, Journal of Physical Chemistry, Journal of the American Chemical Society, Molecular Physics, Nature, Physical Review, Physical Review Letters, Science*, and many others.

Lectures

Several hundred seminars and colloquia delivered throughout the world at major universities, research and industrial laboratories and professional meetings.

10 most important papers of Professor Michele Parrinello

"Unified approach for molecular dynamics and density-functional theory"
R. Car and M. Parrinello
Phys. Rev. Lett. **55**, 2471 (1985), DOI: 10.1103/PhysRevLett.55.2471

"Polymorphic transitions in alkali halides. A molecular dynamics study"
M. Parrinello and A. Rahman
J. de Phys. **42**, C6-511 (1981)

"Escaping free-energy minima"
A. Laio and M. Parrinello
Proc. Natl. Acad. Sci. **99**, 12562 (2002), DOI: 10.1073/pnas.202427399

"QUICKSTEP: Fast and accurate density functional calculations using a mixed Gaussian and plane waves approach"
J. VandeVondele, M. Krack, F. Mohamed, M. Parrinello, T. Chassaing and J. Hutter
Comp. Phys. Comm. **167**, (2), 103-128 (2005)

"The nature of the hydrated excess proton in water"
D. Marx. M. E. Tuckerman, J. Hutter and M. Parrinello
Nature **397**, 601 (1999), DOI: 10.1038/17579

"Well-tempered metadynamics: a smoothly converging and tunable free-energy method"
A. Barducci, G. Bussi and M. Parrinello
Phys. Rev. Lett. **100**, 0206003 (2008)

"Generalized neural-network representation of high-dimensional potential-energy surfaces"
J. Behler and M. Parrinello
Phys. Rev. Lett. **98** (14), 146401 (2007)

"Study of an *F* center in molten KCl"
M. Parrinello and A. Rahman
J. Chem. Phys. **80**, 860 (1984), DOI: 10.1063/1.446740

"Canonical sampling through velocity rescaling"
G. Bussi, D. Donadio and M. Parrinello
J. Chem. Phys. **126**, 014101 (2007)

"Bonding and disorder in liquid silicon"
I. Štich, R. Car and M. Parrinello
Phys. Rev. Lett. **63**, 2240 (1989)

List of publications

Michele Parrinello

Articles

1. "Itinerant theory of ferromagnetism and Hund's-rule coupling"
   T. Arai and M. Parrinello
   Phys. Rev. Lett. **27**, 1226 (1971)

2. "Electron correlations and plasmon dispersion in metals"
   M. Parrinello and M. P. Tosi
   Nuovo Cim. **12B**, 155 (1972)

3. "Electron-ion triplet correlations in liquid metals"
   M. Parrinello and M. P. Tosi
   J. Phys. C **6**, L254 (1973)

4. "Perturbation expansion of the antiferromagnetic ground state"
   M. Parrinello, M. Scirè and T. Arai
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5. "Optical modes in binary alloys"
   M. C. Abramo, M. Parrinello, M. P. Tosi and D. E. Thornton
   Phys. Lett. **43A**, 483 (1973)

6. "Correlations in ionic melts I. Static structure factors and dielectric properties"
   M. C. Abramo, M. Parrinello and M. P. Tosi
   J. Nonmetals **2**, 57 (1973)

7. "Correlations in ionic melts II. Moments of current correlations"
   M. C. Abramo, M. Parrinello and M. P. Tosi
   J. Nonmetals **2**, 67 (1974)

8. "Dynamic structure factors and neutron scattering in molten salts"
   M. C. Abramo, M. Parrinello and M. P. Tosi
   J. Phys. C **7**, 4201 (1974)

9. "Infinite-order cumulant expansion for spins"
   M. Parrinello and T. Arai
   Phys. Rev. B **10**, 265 (1974)

10. "Electronic effects in dynamical structure of liquid metals"
    M. P. Tosi, M. Parrinello and N. H. March
    Nuovo Cim. **23B**, 135 (1974)

11. "Partial structure factors and atomic dynamics in conformal solutions"
M. Parrinello, M. P. Tosi and N. H. March
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C. Caccamo, G. Pizzimenti, M. Parrinello and M. P. Tosi
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16. "Dynamical correlations in the one-component plasma"
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17. "Is the Haeffner effect in liquid metals related to the electrical resistivity of the isotopic mixture?"
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18. "Wavenumber-dependent concentration fluctuations in liquid mixtures"
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20. "Thermodynamics of Wigner crystallization"
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79. "Simulation of electrons in molten salts"
A. Selloni, E. S. Fois, M. Parrinello and R. Car
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80. "Approach to metallic behavior in metal-molten-salt solutions"
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81. "Bonding and disorder in liquid silicon"
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Physica C **162-164**, 771 (1989)

92. "Ab-initio molecular-dynamics of liquid and amorphous semiconductors"
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F. Ancilotto, W. Andreoni, A. Selloni, R. Car and M. Parrinello
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