



PRESS RELEASE

From Dirac to Dreyfus



Michele Parrinello Wins Dreyfus Prize

23 May 2017

Long-time SISSA Professor, ICTP Scientific Council member and Dirac Medallist Michele Parrinello has won the 2017 Dreyfus Prize in the Chemical Sciences, conferred this year in Theoretical and Computational Chemistry. The international prize, awarded biennially, consists of \$250,000, a medal, and a citation.

Parrinello, the first recipient from outside the United States, is honored for his groundbreaking developments of molecular dynamics simulation methodology and associated landmark studies of chemical, material, and biomolecular systems. He is a Professor at Università della Svizzera Italiana and ETH Zurich.



Parrinello shared ICTPs 2009 Dirac Medal with Roberto Car, Department of Chemistry, Princeton University, for developing the *ab initio* simulation method in which they combined the quantum mechanical density functional method for the calculation of the electronic properties of matter with molecular dynamics methods for the Newtonian simulation of atomic motions. The Car-Parrinello method has provided an all-important quantitative understanding of the properties of matter, while also allowing scientists and laymen alike to visualize atoms in motion during physical and chemical processes.

In a press release announcing the prize, Matthew Tirrell, Chair of the Dreyfus Foundation Scientific Affairs Committee, added perspective to Parrinello's work: "Innovations in theoretical and computational chemistry underpin our understanding of biological interactions, chemical dynamics and structure, as well as many beneficial chemical technologies. Michele Parrinello is a giant in the field, whose innovations are widely used in chemistry, biology, materials science, and engineering."

More recently, Parrinello has developed, in collaboration with SISSA Professor Alessandro Laio and others, what is called metadynamics and subsequently announced an efficient variational sampling process. This has allowed the calculation of complicated phenomena such as protein folding, crystallization from a liquid, or the binding of drugs to protein receptors.

Born in Messina, Italy, Parrinello received his Italian *Laurea* in physics from the University of Bologna in 1968 and moved to Trieste in 1977: "Parrinello came with me to the University of Trieste as assistant professor," Erio Tosatti, SISSA Professor Emeritus and ICTP consultant, explains. "He then spent a few years in the United States to work with Aneesur Rahman, the father of molecular dynamics simulations, whom he came to consider his mentor. By the time he returned to Trieste with this new skill, SISSA had opened, and Roberto Car had joined me there as a researcher. Their collaboration led to the well-known Car-Parrinello method which became famous very quickly. In 1985, Parrinello joined SISSA and started receiving very interesting and appealing job offers from abroad: he moved to IBM Zurich, then to Max-Planck in Stuttgart and, eventually, to the ETH Zurich and Università della Svizzera Italiana in Lugano. He has made outstanding contributions to the field of computational physics, chemistry and chemical physics. Some of them have represented a real revolution, as witnessed by many hundreds of papers and countless citations and awards." Tosatti concludes: "We have been friends and colleagues for a very long time. Michele Parrinello is a great man, even besides his monumental scientific achievements. Profound as he is, he is also very strong and enthusiastic, keen to help us in Trieste as well as everyone else at any opportunity."

Parrinello has received many international honors in addition to the Dirac Medal, including the Rahman Prize, the Hewlett-Packard Europhysics Prize (all with Roberto Car), the Schrodinger Medal, the Enrico Fermi Prize, the Swiss Science Prize Marcel Benoist, and the American Chemical Society Award in Theoretical Chemistry. He is a Fellow of the American Physical Society, Socio corrispondente of the Accademia Nazionale dei Lincei (Italy), and a Member of the Royal Society (UK), the European Academy of Sciences, the National Academy of Sciences, the American Academy of Arts and Sciences, and others.



USEFUL LINKS:

The Camille and Henry Dreyfus Foundation: <http://www.dreyfus.org/>

The Dreyfus Prize: <http://dreyfus.org/Prize/prize.shtml>

IMAGE:

Credits: ICTP

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