



MEDIA RELEASE
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ICTP awards prestigious Dirac Medal to simulation experts

The Abdus Salam International Centre for Theoretical Physics has announced that the recipients of its 2009 Dirac Medal are Roberto Car and Michele Parrinello for their revolutionary “molecular dynamics” numerical simulation method for condensed matter.

Their work, known as the Car-Parrinello method, combines quantitative electronic energy calculation, via a theory known as Density Functional Theory (DFT), with Newtonian molecular dynamics simulation of the mechanical motion of atoms and molecules in real time. That method has provided an all-important quantitative understanding of the properties of matter, while also allowing scientists and laymen alike to visualise atoms in motion during physical and chemical processes.

“With this year’s Dirac Medal, ICTP acknowledges the enormous impact the Car-Parrinello method has made on the creation of molecular simulations,” said ICTP Director K. R. Sreenivasan. He added: “This is the first time that the Dirac Medal recognises computational physics properly, the Car-Parrinello method being a major milestone in that area.”

“Up to the 1980s, molecular dynamics simulation was mostly a game. Because it was so very time consuming to calculate the electronic forces that act on atoms, scientists just could not do it fast enough to use them on the fly. So, the simulations were done using invented forces,” said Erio Tosatti, former Acting Director of ICTP and a condensed matter researcher who brought Car and Parrinello to the University of Trieste and to the International School for Advanced Studies (SISSA, next door to ICTP) in the late 1970s.

Car and Parrinello’s clever and elegant trick around the problem treats the DFT electronic parameters as fictitious additional atomic coordinates, and applies Newtonian mechanics to their motion. They published a paper on their method in the November 1985 issue of the journal *Physical Review Letters*; the paper now ranks sixth among the journal’s top cited articles, with a total of 5027 citations. The work created a new paradigm, now an indispensable tool of every computational condensed matter physicist, chemist, and even biologist.

Born in Trieste, Roberto Car is a professor in the Chemistry Department at Princeton University, New Jersey, USA.

Michele Parrinello, who was born in Messina, Italy, is a professor at the Swiss Federal Institute of Technology (ETH Zurich), Switzerland.

ICTP’s Dirac Medal is given in honour of P.A.M. Dirac, one of the greatest physicists of the 20th century and a staunch friend of the Centre. It is awarded annually on Dirac’s birthday, 8 August, to scientists who have made significant contributions to physics. The Medallists also receive a prize of US \$5,000.

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An award ceremony will be held in early 2010.

Based in Trieste, Italy, the Abdus Salam International Centre for Theoretical Physics fosters advanced studies and research in physics and mathematics, especially in developing countries. The Centre operates under a tripartite agreement between the Italian Government, UNESCO and IAEA. Each year about 7000 scientists from around the world visit ICTP for workshops, training and research. For more information, visit the website at <http://www.ictp.it>.

For additional information about the Dirac Medal and a complete list of previous winners, see <http://prizes.ictp.it/Dirac>

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