

Press Release

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For immediate release

Inaugural Walter Kohn Prize Awarded to Chinese Physicist

The first Walter Kohn Prize for quantum-mechanical materials and molecular modeling has been awarded to Professor Yanming Ma, a researcher from Jilin University in Changchun, China. The prize recognizes his development of efficient methods for the determination of crystal structures based on density functional theory and for the prediction of novel phases of materials under high pressure.

The prize was established in March 2016 by the Abdus Salam International Centre for Theoretical Physics (ICTP) and the Quantum ESPRESSO Foundation in honor of Chemistry Nobel Laureate Walter Kohn, a leading condensed matter physicist who developed density functional theory (DFT), a method that drastically reduces the amount of computing power needed to model the properties of complex materials, without compromising the accuracy of a model's simulations. DFT has already had a big impact on a wide variety of fields, including chemistry, molecular physics, medicine and engineering. It also has opened the door to contributions from scientists from disadvantaged countries who have no access to huge supercomputers, due to its low computing costs and the wide availability of open source modeling software.

Professor Ma is a rising star in the quantum-mechanical materials modeling world. His work has featured noteworthy examples of many different aspects of computational materials science: developing novel algorithms, performing virtual experiments, and the *in silico* design of materials with useful properties.

"Yanming Ma is an outstanding scientist, but also an inspiration to students in China," said ICTP condensed matter physicist Sandro Scandolo, who is also a representative member of the Quantum ESPRESSO Foundation. "We are happy that the inaugural prize goes to such an outstanding scientist—it sets the standards high."

"Professor Ma's work has applications as diverse as the design of functional materials—superconductive, superhard, or thermoelectric materials—and the stability of matter at extreme conditions," says Stefano Baroni, professor in the Condensed Matter section at the International School for Advanced Studies (SISSA) and founding director of the Quantum ESPRESSO Foundation. "Not only has Professor Ma authored countless publications, he is also the main developer of an open source software package (nicknamed CALYPSO), thus making his methodology available to a broad scientific audience."

The Quantum ESPRESSO Foundation is the home of some of the most popular and internationally recognized open source codes for quantum-mechanical materials modeling, based on DFT. ICTP regularly organizes schools with the foundation, especially in developing countries.

Professor Ma will receive the Prize at a ceremony to be held 13 January 2017 at ICTP, during the Centre's International Workshop on Computational Physics and Materials Science.

For more details about the prize, visit the Walter Kohn Prize web page (<https://www.ictp.it/about-ictp/prizes-awards/walter-kohn-prize.aspx>).

About ICTP: The Abdus Salam International Centre for Theoretical Physics (ICTP) supports theoretical and applied physics research, as well as training and educational opportunities for scientists from the developing world. Over the past five decades, scientists from 188 countries have made over 140,000 visits to ICTP to learn about the latest findings in their fields, returning to their native countries to share what they have learned. ICTP has been a major force in stemming the scientific brain drain from the developing world. More details at www.ictp.it.

About Quantum ESPRESSO Foundation: The foundation fosters and supports the design, implementation, maintenance, and free dissemination of high-quality, high-performance open-source scientific software for *ab-initio* quantum numerical modeling of materials. More details at <http://foundation.quantum-espresso.org>.

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