NEWS HIGHLIGHTS

First Walter Kohn Prize Awarded

Congratulations to Prof. Yanming Ma

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The first Walter Kohn Prize for quantum-mechanical materials and molecular modeling has been awarded to Professor Yanming Ma, a young 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 on novel phases of materials under high pressure. He 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.

Quantum-mechanical materials modeling is the key to one of the most burgeoning fields of physics: the pursuit of new materials. The search for specialized alternatives to the current building blocks would benefit many applications, in fields as diverse as molecular medicine, space and planetary science, and many many applications, in fields as diverse as molecular medicine, space and planetary science, and many and molecular systems based on the basic laws of physics and chemistry. While inventing or discovering new materials by trial and error in the laboratory takes time, modeling means physicists can predict the properties of whole classes of materials and point chemists towards potentially useful ones. These models

pave the way for attempts at creation of new materials for use in energy harvesting and storage, electronics, nanotechnology, and many others.

The winner of this year's prize, Yanming Ma, is a rising star in the quantum-mechanical materials modeling world. "Professor Ma's research is having a tremendous impact in this field," says Stefano Baroni, professor in the Condensed Matter section at SISSA and director of the Quantum ESPRESSO Foundation, a co-sponsor of the prize. "His work has applications as diverse as the design of functional materials—superconductive, superhard, or thermoelectric materials—and the stability of matter at extreme conditions," Baroni continues. "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."

"One of the hardest problems in physics, chemistry or materials science is to predict the atomic arrangement—the crystal structure of a material—with no prior knowledge apart from the chemical composition,"says Shobhana Narasimhan, member of the Walter Kohn Prize selection committee and Professor of Theoretical Sciences and Dean of Academic Affairs at the Jawaharlal Nehru Centre for Advanced Scientific Research in Bangalore. "Yanming Ma has developed new methods that are a significant step forward in achieving this difficult task. Over the last few years, 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."

The Walter Kohn Prize honors a great founder of the field of materials modeling. Walter Kohn became a leading condensed matter physicist after escaping Nazi Germany in the 1930s for the US. He won a Nobel Prize in Chemistry in 1998 for the creation of density functional theory, or DFT. DFT is a method that drastically reduces the amount of computing power needed to model the properties of complex materials, without compromising on the accuracy of the model. DFT has already had a big impact on a wide variety of fields, but has also opened the door to contributions from scientists without access to huge supercomputers.

These contributions, ingenious algorithms and complex codes that implement DFT, are sometimes expensive commercial products, inaccessible to many. But quite a few of these codes are freely available to all researchers: they are open source, meaning researchers worldwide are free to change and adapt the code to meet ever-changing challenges. The Quantum ESPRESSO Foundation hosts some of the most popular and internationally recognized open source code for quantum-mechanical materials modeling, code based on DFT." Materials modeling is an exceedingly democratic scientific endeavor," says Baroni.

The Walter Kohn Prize aims to celebrate the accomplishments in the field of materials modeling as well as

the drive to include scientists from all over the world and from all resource levels in the scientific process thanks to open source code. Yanming Ma is skillfully accomplishing both, following and building on Kohn's contributions.

Visit the Walter Kohn Prize web page for more details

----Kelsey Calhoun