Tsinghua University
Department of Physics

Thursday Colloquium 2012 Spring

How to discover new materials on the computer:
new methods for crystal structure prediction and computational materials design

Abstract

While most of the known materials have been discovered through experiments, one wonders if theory will ever become capable of leading materials discovery. The evolutionary methodology USPEX has been a major step towards this goal as it provides, given just the chemical composition and pressure / temperature conditions, the stable structure and a set of low-energy metastable structures.
Some of the applications are:
1. New stable high-pressure phase of boron, γ-B. This superhard phase shows a surprising degree of charge transfer between boron sites, which affects many physical properties.
2. Transparent insulating phase of sodium and new phases of calcium, CaLi2, nitrogen.
3. Unusual high-pressure behavior of methane CH4, silane SiH4, germane GeH4 and stannane SnH4.

Many methodological developments happened recently. The method has been extended to molecular crystals, nanoparticles, and crystalline surfaces. It can now deal with systems with up to several hundred atoms in the unit cell. Its extension to variable-composition systems allows simultaneous finding of stable chemical compositions and the corresponding crystal structures in multinary A-B-C⋯ systems. It is now also possible to search for compositions and structures possessing optimal values of a given physical property . For a recent review of this method and its applications, see. I will also discuss recent extension of this method to molecular crystals and a new method – evolutionary metadynamics, which opens new prospects for computational materials discovery.

Speaker

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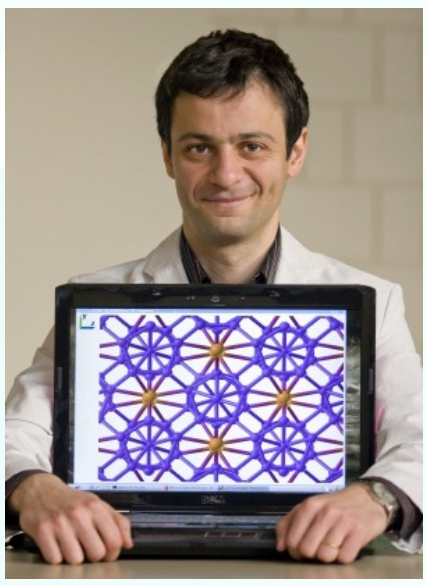

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Zheng Yu-Tong Lecture Hall, New Science Building

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http://www.phys.tsinghua.edu.cn/Colloquium/