Materials Science and Technology Division
Materials Theory Group

"Precise density functional calculations for thousands of atoms"

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11:00 a.m.
4100, Conference Room J-302

Abstract

Quantum mechanical calculations based on density-functional theory provide an increasingly powerful tool to understand the properties of materials for advanced 21st century applications. Standard algorithms for such calculations cannot treat systems with thousands of atoms because the computing times scale as the third power of the number of atoms.

In the talk I will present our newly developed code KKRnano which does not suffer from this bottleneck. I will describe the basic principles of our algorithm and show that KKRnano efficiently runs on supercomputers with many thousand processors. I will demonstrate that no compromise on accuracy must be made if KKRnano is operated in the normal mode with computing times which scale quadratically with the number of atoms. Calculations with linearly increasing effort are also possible if small total-energy changes of a few meV per atom are tolerated. From our first applications to systems with several thousand atoms I will discuss results for a dilute magnetic semiconductor (Gd in GaN), a crystalline phase-change material (GeSb2Te4) and a nanocolumnar konbu-phase structure (ZnCrTe).

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