



INTERDISCIPLINARY CENTRE FOR
ADVANCED MATERIALS SIMULATION

ICAMS Seminar

Prof. Matthieu Verstraete

Universite de Liège, Belgium

Monday, January 14, 4:30 p.m.
ICAMS seminar room 0.08

"Ab initio prediction of thermoelectrical properties of materials

The post-petroleum economy which is developing in the world necessitates new materials for the production, conversion, and storage of energy. The most developed and long-standing technologies are wind and solar, but a crucial role can be played by thermoelectrical materials, which convert heat currents into electrical ones, or vice versa. They can function either to recuperate waste heat or to provide solid-state heating and cooling devices, with the best reliability on the market, e.g. in deep space craft which are too far from the sun, and subsist on a radioactive heat source coupled to thermoelectrical devices. Profound challenges remain, however, in making thermoelectrical materials efficient enough to compete with other energy sources, but over the past 15 year significant new paradigms have been opened up in nanostructuring and intelligent doping. I will present our developments to calculate the transport properties of materials in a purely ab initio framework (i.e. without using a relaxation time approximation), and focus on a few recent materials we have studied.

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