The 137th MANA Special Seminar

Density functional based global geometry optimization and their application to clusters with cage-like structure

Chair: Dr. Yoshitaka Tateyama (MANA Independent Scientist)

Professor Stefan Goedecker

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Global geometry optimization allows to find the global minimum of the potential energy surface of condensed matter systems. The ground state structure of molecules, nano-systems and crystalline materials can thus be predicted. I will first introduce the two essential methodological ingredients of our global geometry optimization, namely the minima hopping algorithm and the BigDFT density functional (DFT) program which uses wavelets as basis functions. I will next show that global optimization on the DFT potential energy landscape is easier than on the potential energy landscape of more approximate schemes such as force fields. Finally I will show structures that were obtained by global optimization for charged clusters, endohedral metal doped silicon clusters, boron fullerenes and model crystalline structures.

Venue: **Seminar Room #431, MANA Bldg.**

Date: **Apr 9th Friday** ***Time:*** **15:30-16:15**

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