The Computational Materials Science Unit Colloquium

理論計算科学ユニットコロキウム

Date & Time: February 10th (Tue.) 3:00pm – 5:00pm

Place: Seminar room, Theoretical Research Building, Namiki site

Speaker: Prof. Michael J. Gillan,
London Centre for Nanotechnology,
University College London, UK

Title

Accurate energetics of methane hydrate and ice structures from quantum Monte Carlo and quantum chemistry

Abstract

Methane hydrate may be a very important future source of energy, because the amount of methane believed to exist in deposits of methane hydrate is greater than all the methane in conventional reserves of natural gas. In addition, methane hydrate is important in the oil industry and may play a role in climate change. Computer simulation work on the energetics of gas hydrates has been reported for many years. Most of this work has been based on empirical force fields, but there is also work based on density functional theory (DFT). Unfortunately, it has become clear recently that commonly used DFT approximations are very inaccurate, partly because of difficulties in describing van der Waals dispersion. This talk will present current work in which quantum Monte Carlo techniques are being used to establish very accurate benchmarks for the energetics of the methane hydrate crystal and also for methane-water clusters. Comparison of DFT approximations with these benchmarks indicates that DFT errors are closely related to the large errors found in describing ice structures. It will be shown that the errors arise not only from dispersion, but also from the description of quantum exchange effects.

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