Institut für Theoretische Physik
Center for Computational Materials Science
TU WIEN

SEMINAR AUS THEORETISCHER PHYSIK

Statistische Mechanik und Theorie der Kondensierten Materie

Laura Filion

Soft Condensed Matter

Debye Institute for NanoMaterials Science
Utrecht University, The Netherlands

Prediction and stability analysis of binary hard-sphere crystal structures

Ort: Seminarraum 136, Wiedner Hauptstraße 8-10, 1040 Wien
Zeit: Mittwoch, 22.7.2009, 16 Uhr s.t.

The ability of atomic, colloidal, and nanoparticle systems to self organize into crystal structures makes the prediction of crystal structures in these systems an important challenge for science. In a recent Nature Review Article, Scott Woodley and Richard Crow claim The prediction of structure at the atomic level is one of the most fundamental challenges in condensed matter science.Thus it is unsurprising that the subject has received much attention from the scientific community over the last several decades. The question itself is deceivingly simple: assuming that the underlying interaction between constituent particles is known, which crystal structures are stable. In this talk we describe a method based on a combination of a genetic algorithm and Monte Carlo simulations to predict close-packed crystal structures in hard-core systems. We apply the method to study binary hard-sphere systems and use it to predict the binary structures in a mixture of large and small hard spheres with various stoichiometries and diameters ratios between 0.4 and 0.84. Additionally, we present the results of computer simulations studying the stability of the predicted AB and AB_2 stoichiometric binary mixtures of hard spheres for size ratios 0.74-0.85.

Gerhard Kahl (58801/13632)