

Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Sampling of stable and metastable cluster structures by a first-principles Monte Carlo approach RALF GEHRKE, KARSTEN REUTER, Fritz-Haber-Institut, Faradayweg 4-6, D-14195 Berlin — Size-selected nano-scale atomic clusters are now systematically becoming accessible in experiment, but characterizing their ground-state and metastable isomer ensemble averages from first principles requires a global and local exploration of vast configuration spaces. We here explore a first-principles Monte Carlo scheme to efficiently sample the minima of the corresponding total energy landscapes. The energetics is obtained at the density-functional theory level, using an all-electron local orbital based first principles code,¹ which allows to switch seamlessly from minimal size effective tight-binding like to meV-level chemically accurate basis sets within a single fundamental framework. The sampling strategies rely on basin hopping, using different schemes to create new trial structures. We demonstrate the reliability and performance of the approach for Cu and Si clusters, discussing in particular the scaling behaviour with the system size.

¹M. Scheffler and V. Blum; R. Gehrke, F. Hanke, P. Havu, V. Havu, X. Ren, K. Reuter, P. Rinke, A. Sanfilippo, A. Tkatchenko, The FHI - Ab Initio Molecular Simulations (aims) project, www.fhi-berlin.mpg.de/aims

Ralf Gehrke
Fritz-Haber-Institut, Faradayweg 4-6, D-14195 Berlin

Date submitted: 23 Nov 2007

Electronic form version 1.4