

Clusters of Transition Metal Atoms at Non-zero Temperatures

Zacharias G. Fthenakis^{a,b}, Antonios N. Andriotis^a, Madhu Menon^c

^a*Institute of Electronic Structure and Laser, P.O. Box 1527, Heraklion-Crete 71110, Greece*

^b*Dept of Physics, University of Crete, Heraklion-Crete, 71110, Greece*

^c*Dept of Physics and Astronomy and Center for Computational Sciences, Univ. of Kentucky,
Lexington, KY40506-0055*

Abstract

A new method is presented which allows one to study the effect of temperature on the structural and magnetic properties of clusters of transition metal atoms. The method is based on our previously reported Tight Binding Molecular Dynamics method (see Phys. Rev. **B57**, 10069 (1998)), the Nose-bath and the Multiple Histogram approximations. Preliminary results obtained with the proposed method for the variation of structural and magnetic properties with temperature as well as the caloric curves of Ni_n clusters will be presented and compared with reported results obtained by other methods.