Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Vibrational and thermodynamic properties of transition-metal nanoclusters[1] VALERI G. GRIGORYAN, MICHAEL SPRINGBORG, Physical and Theoretical Chemistry, University of Saarland, Germany — The knowledge of the vibrational spectrum of a cluster, which is the fingerprint of its structure, is necessary for the development of thermodynamics of clusters (melting, heat capacity, solid-solid structural transitions) and for the understanding of experimental vibrational spectra. In summary, the full vibrational spectrum of Ni_N and Cu_N nanoclusters with N from 2 to 150 atoms has been determined using the analytical expression of the embedded-atom method (EAM) for the *force-constant tensor* for the first time. In the determination of the spectra we have employed the global-minimum structures obtained in our previous unbiased EAM studies (see e.g. Physical Review B, 2004; 2006). Furthermore, using those spectra and the superposition approximation, the thermodynamic properties of the clusters have been calculated quantum mechanically, including their heat capacity and solid-solid transition temperatures for several structural changes in the Ni and Cu clusters. Both the vibrational spectrum and the thermodynamic functions show strong cluster-size effects. We emphasized that our approach is general. It is based only on the (common) EAM form of the total energy and applicable to many other many-body potentials.

[1]This work was supported by the DFG through Project No. Sp439/23-1

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Date submitted: 08 Nov 2012 Electronic form version 1.4