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Vibrational Dynamics and Thermodynamics of AgCu nanoparticles[1] ABDELKADER KARA, HANDAN YILDIRIM, TALAT S. RAHMAN, Physics Department, Kansas State University, RICARDO FERRANDO, INFM and IMEM-CNR, Dipartimento di Fisica dellUniversita' di Genova, via Dodecaneso 33, 16146 Genova, Italy — We present results of a systematic study of the structure, vibrational dynamics and thermodynamics of Ag_nCu_{34-n}nanoparticles including. The starting structure were generated using a structural optimization using a genetic algorithm [1]. Using the embedded atom method potentials, we have calculated the vibrational densities of states for all stoichiometries and the corresponding vibrational free energies, in the harmonic approximations. At 300K, the vibrational free energy is found to behave linearly with the increasing number of Ag atoms in the nanoparticles. The vibrational contributions to the free energy increase from 5.5% for Ag_0Cu_{34} to 8.3% $Ag_{34}Cu_0$. Selected force constants for several nanoparticles were calculated using density functional theory (DFT) and were found to be very close to those determined using EAM potentials. [1] G. Rossi, A. Rapallo, C. Mottet, A. Fortunelli, F. Baletto and R. Ferrando Phys. Rev. Lett, **93**, 105503 (2004)

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