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***Ab initio* vibrational dynamics of $Ag_{27}Cu_7$ nanoalloy.** MARISOL ALCANTARA ORTIGOZA, University of Central Florida, ROLF HEID, KLAUS P. BOHNEN, Forschungszentrum Karlsruhe (IFP), TALAT S. RAHMAN, University of Central Florida — We have carried out calculations of the vibrational dynamics of the 34-atom nanoalloy, $Ag_{27}Cu_7$, using density functional perturbation theory, which furnishes a powerful and reliable method to asses the linear response of the charge density to ionic perturbations. We find that the D_{5h} core-shell structure of $Ag_{27}Cu_7$ [1,2] is dynamically stable, since all modes have non-zero frequencies affirming that the structure does not surrender itself to structural transitions as a result of the small perturbations in the charge density led by vibrations. The phonons of $Ag_{27}Cu_7$ range from 2.6 to 28.5 meV and are relatively evenly distributed. There are, however, three $\sim$3.0 meV gaps between 2.8-5.6, 15.0-18.7, and 23.6-26.8 meV. In modes whose frequency is below 7.0 meV, Ag atoms participate the most while Cu atoms show a very small displacement. The opposite is true for four modes whose frequency is above 24 meV. We present the displacement patterns of the main modes and find the mode with highest energy to be a radial *breathing* mode of Cu atoms with respect to the center of the cluster. [1] G. Rossi *et al.*, PRL. **93**, 105503 (2004), [2] M. Alcántara Ortigoza and T. S. Rahman, PRB **77**, 195404 (2008). Work supported in part by U.S. DOE under Grant DE-FG02-07ER46354.

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