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Linear and Nonlinear Optical Properties of GaN Nanoclusters
SHASHI KARNA, US Army Research Lab, Weapons and Materials Directorate, ANDREW PINEDA, USAF Research Lab, Space Vehicles Directorate, 3550 Aberdeen Avenue, SE, Kirtland AFB, 87117-5776 — The linear and nonlinear optical (NLO) properties of III-V binary semiconductors have been a subject of active research since the late 1960s. Recent advancements in (a) experimental techniques to fabricate/produce stable nanometer-size binary atomic clusters composed of group III and group V elements and (b) techniques and tools to probe response properties of nano-scale objects, have attracted a great deal of attention in the linear and NLO properties of III-V nanoclusters due to their potential applications in future technologies. An important issue in a bottom-up approach to fabricating nanoclusters for future technological applications is an understanding of the evolution of response properties with cluster size. In order to develop such an understanding, we have undertaken a systematic study of the electronic and geometrical structures and the optical properties of III-V nanoclusters by first-principles *ab initio* time-dependent Hartree-Fock calculations. In this talk, we present the results of our first-principles quantum mechanical studies of the electronic structure, stability, and linear and NLO properties of Ga_mN_n atomic clusters, with values of m and n ranging between 1and 17. Our calculated results suggest that the linear and NLO properties both exhibit strong dependence on the cluster size and shape. However, the size-dependence is more pronounced for the NLO properties than that for the linear optical properties.

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