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***Ab initio* investigation of the electronic properties of Hg_mTe_n clusters**[1] SACHIN NANAVATI, C-DAC, University of Pune, Pune 411007, India, VIJAY KUMAR, Dr. Vijay Kumar Foundation, 1969, Sector 4, Gurgaon 122001, India; Center for Informatics, School of Natural Sciences, Shiv Nadar University, UP India, RAVINDRA PANDEY, Department of Physics, Michigan Technological University, Houghton, MI 49931, USA, AMBESH DIXIT, Indian Institute of Technology Jodhpur — Nanostructured HgTe quantum dots have attracted attention due to their potential applications in novel mid-infrared (3 – 5 μm) wavelength photodetectors and other optoelectronic applications. HgTe bulk material is a semimetal with bandgap $\sim$ -0.3 eV, however at nanoscale, we observe drastic changes in the optical and electronic properties such as band gap opening, that makes it possible for engineering optoelectronic properties. We investigated the structural, optical, and electronic properties of Hg_mTe_n (m = n = 12, 13, 33, and 34) nanoparticles using density functional theory and the pseudopotential method within the generalized gradient approximation. The structures are relaxed to achieve the stable configurations and corresponding electronic properties are calculated. We investigated the density of states, energy gap between the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO), binding energy, and the Hg-Te bond length variation as a function of the cluster size. We will discuss the changes in the electronic structure and optical properties for these clusters with respect to the cluster size variation.

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