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Structural and optical properties of mercury chalcogenide HgSxSe1-x and HgSxTe1-x nanocrystals: Atomistic tight-binding theory

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The structural and optical properties of the mercury chalcogenide HgSxSe1-x and HgSxTe1-x nanocrystals with zinc-blende structure are analyzed using the sp3s* empirical tight-binding method. We calculate the single-particle spectra, band gaps, charge densities, density of state (DOS), electron-hole interaction and optical properties as a function of diameters and alloying concentrations (x). The computations highlight that these natural properties are sensitive with diameters and alloying contents (x) of HgSxSe1-x and HgSxTe1-x nanocrystals. Finally, the scheme is expected to provide the detailed information in electrical and optical properties of HgSxSe1-x and HgSxTe1-x nanocrystals with the aim to implement them as the novel nanoelectronic devices.

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