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Computational study of lead selenide doped with group IIIA elements

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Lead selenide (PbSe) is a semiconductor of the cubic structure whose bandgap is 0,27 eV. It belongs to a group of essential materials for developing uncooled mid-IR detectors. This material also proved to be an excellent thermoelectric, offering a few advantages compared to other materials. It is also worth mentioning that doping can readily modify its properties. In this work, we have studied the structural and electronic properties of PbSe doped with IIIA group elements. Applying density functional theory calculations, we have investigated how the introduction of mentioned elements into the structure of PbSe influences characteristic bond lengths and cell parameters, band structure and density of states. Charge distribution of doped PbSe was also under consideration through calculations of electron density difference, while effective screening medium calculations were performed to understand the properties of PbSe surface upon incorporating mentioned elements.

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