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High pressure properties of I-III-VI_2 compounds from ab initio calculation

Thursday, May 21, 2015 8:00 AM (3 hours)

Ab initio calculation based on density functional theory were performed for studying high-pressure phases and electronic properties of I-III-VI_2 compounds. Thermodynamic properties of a solid system were calculated by using LDA and PBE functionals. Stability of high pressure structures of I-III-VI_2 compounds were determined by comparing the lowest enthalpies. The high-pressure properties such as lattice parameter, electron density and elastic constant were investigated up to 200 GPa. Stability of high pressure structures were observed by studying the phonon dispersion relation.

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