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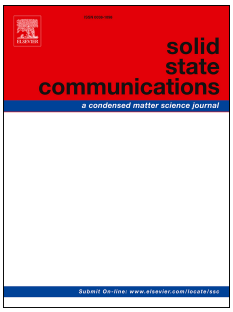

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Electron Transport in NH_3/NO_2 Sensed Buckled Antimonene

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Abstract

The structural and electronic properties of buckled antimonene have been analysed using density functional theory based ab-initio approach. Geometrical parameters in terms of bond length and bond angle are found close to the single ruffle mono-layer of rhombohedral antimony. Inter-frontier orbital analyses suggest localization of lone pair electrons at each atomic centre. Phonon dispersion along with high symmetry point of Brillouin zone does not signify any soft mode. With an electronic band gap of 1.8eV, the quasi-2D nano-surface has been further explored for NH_3/NO_2 molecules sensing and qualities of interaction between NH_3/ NO_2 gas and antimonene scrutinized in terms of electronic charges transfer. A current-voltage characteristic has also been analysed, using Non Equilibrium Green's function (NEGF), for antimonene, in presence of incoming NH_3/ NO_2 molecules.

Keywords: Antimonene, sensor, DFT, Adsorption energy, Bandstructure, Transmission Spectra