Structural and electronic properties of the incommensurate Bi-III phase

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Bismuth, one of the most intriguing elements, was found to adopt an incommensurate host-guest structure at moderately high pressures and ambient temperature [1]. Higher resolution measurements revealed periodic modulations of the atoms in respect to their basic structure [2], which suggest a stabilizing mechanism for this structure, based on the interactions between the host and the guest sub-lattices. We present a comprehensive computational study of the incommensurate Bi-III phase within the framework of DFT, using several commensurate approximations. The detailed structure of the phase is obtained, including the ratio between the host and the guest lattice constants and the atomic modulations, all in good agreement with the experiments. The pressure dependence and stability range of the host-guest phase are also successfully reproduced. Spin-orbit coupling effects were studied by using fully-relativistic pseudopotential, and their influence on the electronic structure and the equation-of-state is discussed.

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