Single isovalent impurity calculations: Bi in InP

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Recently dillute III-V-bismides have attracted attention due to their potential applications in optoelectronic devices [1]. Despite the growing interest few electronic calculations have been done on dillute Bi in InP. In this work we study the local density of states (LDOS) of a single Bi impurity atom in InP host. We use the Koster-Slater technique to calculate the impurity Green's function [2] together with an empirical spds* tight binding Hamiltonian [3]. By taking the imaginary part of the calculated Green's function we obtain the spatial structure of the LDOS which can be compared with cross-sectional scanning tunneling microscopy (X-STM) measurements.

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