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Ab Initio Calculation of Electronic Properties in Si:H ALVARO POSADA-AMARILLAS, Dept de Investigacion en Fisica, Universidad de Sonora, ROBERTO NUNEZ-GONZALEZ, Dept de Matematicas, Universidad de Sonora — In this work we calculate the electronic structure of crystalline silicon with monatomic hydrogen, using the LAPW method within the DFT framework. The density of states, charge density and stable configuration of Si in bond-center (BC) and tetrahedral (Td) sites are calculated. Supercells are used in order to study several hydrogen concentrations, finding a metallic behavior in all cases. Important contributions at the Fermi level are due to hydrogen, and the Td site is the most stable for hydrogen concentrations on the order of 50%.

Alvaro Posada-Amarillas
Dept de Investigacion en Fisica, Universidad de Sonora

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