

Molecular modelling of lithium intercalation in 1T-TiS₂

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The electronic structure of 1T-TiS₂ intercalated with lithium is analysed within a molecular approach that uses a finite-size cluster to represent the solid. Electronic descriptors such as the electronic chemical potential, bond order and the density of states are used to discuss the bonding properties and migration of lithium within the layered lattice. A detailed analysis of the electronic structure reveals the major role of local interactions involved in the electronic polarization of the impurity's environment. The results compare well with the available experimental data.