The electronic chemical potential as a basis for a cluster model approximation for intercalation of Li in 1T - TiS2

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The representation of the electronic structure of intercalated 1T - TiS2 with lithium by a cluster approximation is discussed. The electronic chemical potential, defined in the context of density functional theory, is used as a criterion to determine the minimal units that retain the major electronic properties of the actual solid. The results indicate that a structure containing 3-4 hexagonal unit cells of TiS2, with an octahedral coordination around the transition metal, is good enough to reproduce the major features of the electronic structure of the infinite layered solid. Analysis of the valence and conducting bands shows good qualitative agreement with band theory calculations. A partial electron transfer from Li to the lattice is predicted, in good agreement with experimental NMR data for this system.