

# A model for the charge capacity of 1T-TiS<sub>2</sub> intercalated with Li

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The variation of the charge capacity of a double-layer 1T-TiS<sub>2</sub> model system upon increasing intercalation with lithium is examined at a molecular level. The charge capacity is modeled through the global hardness index of density functional theory. The results obtained qualitatively reproduce the experimental trend observed in the voltage-composition variation curve in this system.

Comparison with previous theoretical models show that the present approach may give a more complete information about the double-layer capacitance, since it takes into account the lithium ionicity and the host-guest specific interactions. © 1995 John Wiley & Sons, Inc. Copyright © 1995

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