

Quantum chemical model for lithium electrochemical intercalation into molybdenum disulfide

Mendizábal, Fernando

Santa Ana, María Angélica

Benavente, Eglantina

González, Guillermo

Voltage- and incremental charge capacity-composition curves for the electrochemical formation of intercalates Li_xMoS_2 were analyzed at the molecular level by developing a quantum chemical model focused on the variation of the electron chemical potential. Experimentally observed trends of the charge capacity in the range $0 < x < 0.6$ are successfully described by the global hardness index as defined within the density functional theory. Contrasting with classical descriptions like the gas lattice model assuming complete lithium-MoS₂ one electron transfer, proposed model leads, agreeing with previous experimental evidence, to a system in which electron density is partially retained in the lithium atom. The model permits moreover to identify a sequence of octahedral and tetrahedral sites as the more favorable migration pathway for the diffusion of lithium through the interlaminar space.