

Redox potentials and diffusion of lithium in lamellar compounds

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Thermodynamic and dynamic properties of intercalation products of lithium into MoS₂ are strongly determined by the coordination of lithium in the interlamellar spaces. Lithium redox potentials as well as lithium diffusion coefficients in MoS₂ pure, exfoliated, as well as in compounds where lithium is co-intercalated with the polymeric electron pair donors, poly(ethylene oxide) and poly-acrylonitrile, and discrete species, OH⁻ ions and secondary amines, were analyzed comparatively. Reduction potentials in pure or exfoliated MoS₂ are always much lower than those observed in lithium-donor co-intercalates. Thus, donors appear to effectively stabilize higher lithium oxidation states. The donors also influence lithium migration properties, with lithium diffusion coefficients in general higher than in pure MoS₂. Lithium diffusion activation energy in pure MoS₂ is constant in a relatively large lithium concentration range, while for co-intercalates it often depends on lithium intercalation deg