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Lithiation of Ag_xMnO_2: Insights from first principles MERZUK KALTAK, MARIVI FERNANDEZ-SERRA, State Univ of NY- Stony Brook, MARK HYBERTSEN, Center for Functional Nanomaterials, Brookhaven National Laboratory — Stable electrode materials being able to capture high lithium concentrations are attracting considerable interest in science as well as industry. Recently hollandite α-MnO_2 based structures are moving into the focus of electrochemists and are considered to be promising electrodes for increasing the capacity and efficiency of rechargeable lithium batteries. These favorable properties are mainly due to the tunnel structure consisting out of stacked 1×1 and 2×2 MnO_2 octahedra in the z-axis. It has been shown that large ions such as silver or potassium can stabilize and increase the cyclicity of pure hollandite α-MnO_2 considerably. In this work we present new insights from first principles for lithiated silver hollandite $Li_yAg_xMnO_2$ and demonstrate that the formation of oxygen vacancies play an important role for lithium diffusion.

Merzuk Kaltak
State Univ of NY- Stony Brook

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