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Phase stability and Jahn-Teller distortion in doped lithiated manganese oxides: A LSDA+U study RAJENDRA PRASAD, NITYA NATH SHUKLA, Indian Institute of Technology, Kanpur, ROY BENEDEK, Argonne National Laboratory — We discuss how the rhombohedral phase of lithiated manganese oxide can be stabilized by doping with various impurities. Our study is based on LSDA+U calculations as implemented in the VASP code. We have considered rhombohedral and monoclinic phases using a supercell of 16 atoms. Our results are based on total energy calculations for 25% dopant concentration and pure lithiated manganese oxide. Several dopants such as Co, Fe, Ni, Mg and Zn are considered. We find that oxidation state of the dopant plays an important role in suppressing the Jahn-Teller distortion. Divalent impurities are found to be most effective. The effect of including U in the calculation is discussed.

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