Doped manganites as cathodes for sodium-ion batteries: a self-consistent DFT+U study.

D. Corona[1], F. Buonocore[2], and O. Pulci[1]

[1]*Department of Physics, University of Rome Tor Vergata, and INFN, Via della Ricerca Scientifica 1, 00133 Rome, Italy.*

[2]*Energy Technologies and Renewable Sources Department, ENEA, Casaccia Research Centre, 00123, Rome, Italy.*

domenico.corona@roma2.infn.it

Sodium-ion batteries share similarities with the well-established lithium-ion batteries currently in widespread use; in fact, analogously to lithium-ion positive electrodes, sodium-ion cathodes store sodium through an intercalation mechanism. Cathodes based on P2-Na_xTMO_2 crystals, i.e., sodium-based layered transition-metal oxides (LTMOs), have attracted growing interest owing to their high potential and capacity. However, the geometric structure of LTMOs may undergo a Jahn-Teller distortion during charge/discharge cycles. Doping has proven effective in stabilizing the P2 geometric structure improving the cycling stability by limiting structural transitions as well as delaying them at higher voltages.

Ab-initio calculations within the Quantum ESPRESSO suite are employed to determine the optimal dopants, the total energy of the system, and estimate the sodium-ion intercalation potential. The structural and electronic properties of doped LTMOs are investigated at a GGA+U level of theory, where the on-site Hubbard U parameters are evaluated self-consistently using linear-response theory, so to realistically include the screening from the environment which is crucial for quantitatively predictive calculations on novel materials.

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