Atomistic design of layered cathode materials for Na-Ion Batteries

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Sodium-ions batteries (NIBs) are very promising substitutes for Lithium-ions rechargeable batteries (LIBs) because of the larger worldwide diffusion and lower production cost of Sodium as compared to Lithium. Beside major safety, good performances and cheaper costs, the same technology and manufacturing already developed for LIBs can be directly applied to NIBs without extra costs. The drawback of NIBs is the lower capacity and duration in terms of cycling life. One of the reasons is that, when Na ions concentration decreases in the cathode of the batteries, the Jahn-Teller effect induces a distortion of the geometry that makes the ions transition irreversible. From these considerations, the realization of stable high-capacity Na ions-based cathodes emerges as an undoubtedly challenging task and calls for in-depth multi-disciplinary investigation by chemists, experimental physicists and condensed matter theoreticians. In this scenario, predictive ab initio simulations could bring valuable insights for the development of this field. In this talk we will report out recent results into investigating the properties of novel Na-based cathodes (stability, electronic properties, redox potentials) by means of first principles DFT calculations. Several approaches (GGA, self-consistent LDA+U, hybrid exchange and correlation functionals) will be used. Such approaches are used to understand the role of doping on the structural stability, by substituting some of the Mn atoms with transition-metal ions and the Na ions diffusion inside cathodes.