High-Throughput Automatic Workflow for 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 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 the automatic workflow of ab initio calculations for cathode materials based on layered metal oxides that has been set up to determine the energetic properties of crystalline structures as the doping level and the doping species change, to generate a database for the search for the most stable crystal compositions. The computational power of ENEA's CRESCO cluster was used to accurately simulate and explore numerous crystalline compositions and configurations using this workflow. The results of the calculations are collected automatically and recorded in a database managed by ENEA.