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Joint computational and experimental investigation of materials for Fluoride-Ion Batteries

The uneven distribution, limited abundance and difficult extraction of lithium pose significant threats to the future sustainability of rechargeable batteries industry supply chain, and makes the development of alternative technologies a pressing need. Fluoride-ion batteries (FIBs) exhibit higher theoretical performances and lower costs than their lithium-ion counterparts, but the technology is in its infancy and much effort is still needed to develop electrodes and electrolytes that can make FIBs commercially viable.
In this work we investigate the electrochemical properties of some electrode and electrolyte prospect materials through a synergic combination of Raman spectroscopy and ab-initio modeling. While Ni-based Ruddlesden-Popper perovskites represent interesting electrode systems with doping-tunable F- diffusion rates, the selection of room-temperature conductive solid-state electrolytes proves more difficult. Current studies, focused on a couple of different families of materials, are searching for crystals that exhibit both significant ionic conductivity and an extended room-temperature electrochemical stability window.

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