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Metal ion exchange mediated structural modulation in layered perovskites: Step towards next-generation energy-efficient materials

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An important challenge of this century is to focus on the production of renewable and sustainable energy, which thrives on research in the development of photovoltaic (PV) materials [1] (solar energy to electricity) and photoelectrochemical (PEC) water-splitting materials (solar energy into chemical energy) [2]. Among the various PV and PEC materials, perovskite structured oxides (ABO3 where A=alkaline or rare-earth metals; B=transition metals) are promising candidates because of their structural and compositional flexibility, excellent stability, and superior optical and electrical properties. Compared to normal perovskites, the layered derivatives show superior photocatalytic performance because they facilitate charge separation due to their unique flexible layered structures. Layered perovskites consist of a perovskite block (ABO3) of varying unit cell thickness n sandwiched between metal oxide layers to form a natural superlattice such as (i) Ruddlesden Popper (RP), (AO)(ABO3)n -alternating perovskite slabs displaced by (1/2,1/2) translation or (ii) Dion Jacobson (DJ), M+1A(n-1)BnO(3n+1) - displacement of the perovskite slabs is either (1/2,0) or is absent. Also, the octahedral rotations or tilts associated with the disconnected octahedra in layered (n = 2) compounds cooperatively give rise to a net polar symmetry with macroscopic polarization known as hybrid improper ferroelectricity (HIF) [3]. In the layered perovskites, the DJ phases offer feasibility for structural modulation via cation-exchange reactions, which stabilizes most metastable phases, which are unpreparable by the direct synthesis routes. In the present study, a series of n = 2 DJ oxides RNdB2O7 (R=Rb, Cs, Na, K and B=Nb, Ta) has been synthesized. (Rb,Cs)NdNb2O7 and (Rb,Cs)NdTa2O7 were synthesized using solid-state reaction, whereas NaNdTa2O7, KNdTa2O7 were obtained by cation-exchange reaction (Fig. 1). The synthesized compounds were analyzed through powder X-ray diffraction. Dion–Jacobson perovskites can also facilitate exfoliation into 2D nanosheets, and finally, the layer-by-layer engineering of 2D perovskite nanosheets has a great potential for next-generation energy-efficient devices [4].

Fig. 1 Cation Exchange in DJ compound

Author: PRASANNAN, Neenu (IFIMUP, University of Porto)

Co-authors: Mr CESÁRIO, António (IFIMUP); Mr SILVA DE SOUSA, Pedro (IFIMUP); Dr LORA DA SILVA, Estelina (IFIMUP); Prof. ARAÚJO, Araujo Joao Pedro (IFIMIP); Dr LOPES, Armandina (IFIMUP)

Presenter: PRASANNAN, Neenu (IFIMUP, University of Porto)

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