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Phase transition pathway of Sr3Hf2O7

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We present an ab-initio study performed by means of Density Functional Theory (DFT), group-subgroup symmetry analysis and lattice dynamics to direct the design of Ruddelstein-Popper (RP) perovskite systems with novel properties and therefore aid experimental synthesis. From this study it is possible to obtain information regarding the structural properties and local landscapes, such as octahedra rotations, tilts and distortions which occur during a structural phase transition, and that will aid and complement the interpretation of analysis performed through Perturbed Angular Correlation (PAC) radioactive nuclear techniques.
More specifically we focus our study on the Sr3Hf2O7 system characterized by a high-temperature I4/mmm (S.G. 139) centrosymmetric structure and a ground-state Cmc21 (S. G. 36) ferroelectric system. We have probed potential candidates that may form the pathway transition through the I4/mmm ⟹ Cmc21 the structural phase transitions, and which were obtained through group-theoretical analysis, namely Fmm2 (S.G. 42), Cmca (S.G. 64) and Cmcm (S.G. 63). These phases were then analyzed to probe the electronic properties (band gap widths and partial density of states; PDoS), electric field gradients and dynamical stabilities through lattice dynamics. We found that the band gaps increase has the symmetry of the systems decrease, with the ground-state structure presenting the largest gap width (˜5.95 eV). By probing the PDoS we observe a direct relation regarding the tilts and rotations of the O perovskite cages as the transition occurs; these show large variations mostly for the O p-states which contribute mostly to the valence band maximum and consistent with the distortions from the high-symmetry to the low-symmetry phases. Moreover we also show that the asymmetry parameter, η, of the electric field gradients tend to vary as the transition occurs, namely these increase through the transition pathway, with Cmc21 evidencing largest values of the order of 0.704, 0.704 and 0.944 for the Hf, Sr1 and Sr2 sites, respectively.

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