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Ab initio calculations on cadmium-based multiferroics

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In multiferroic systems, the coupling between electric and magnetic properties gives birth to new tactics to conceive novel technological architectures. The mechanism of ferroelectricity is crucial to materials with high magnetoelectric coupling. As a result, the discovery of hybrid improper ferroelectric (HIF) materials opened new routes for multiferroics design. The Ruddlesden-Popper (RP) and double perovskite (DP) structures are possible HIF compounds, and the RP Ca3Mn2O7 is a prototype for the construction of new HIF materials.
Recently, perturbed angular correlations (PAC) spectroscopy combined with density functional theory (DFT) calculations depicted the relations between the electric field gradient and the structural phase transitions in Ca3B2O7 (B = Ti, Mn) systems. PAC experiments used 111mCd probes that, because of the similar ionic radii and same cation valence charge as Ca, easily substitute Ca ions in Ca3B2O7. Theoretical calculations have shown that Cd is stable at the rocksalt site of Ca3B2O7, leading to the question of how much Cd can Ca3B2O7 incorporate.
Here, we used ab initio calculations to investigate the effect of substituting Ca by Cd in several RP and DP systems. Our results show that enthalpy relations favor the decomposition of Cd-based RP compounds, indicating that experimental synthesis may be nontrivial. Although pure Cd-related RP compounds are not stable, RP Ca3B2O7 (B = Ti, Mn) systems admit the incorporation of certain percentages of Cd replacing Ca. Having a significant impact on the ferroelectric properties, these chemical substitutions can be used to engineer RP and DP materials, increasing their applicability range as ferroelectric and piezoelectric materials [1,2].

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References:
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Scientific Area

Quantum materials and quantum technogies

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