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Ab-initio Study on CsNdNb2O7 and CsLaNb2O7 Dion-Jacobson Perovskites

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In the pursuit of novel and highly efficient multiferroic materials, significant exploration has unfolded during the last decades. These materials, characterized by their ability to exhibit a myriad of intriguing phenomena, hold promise in enabling the electrical manipulation of magnetic degrees of freedom, thus offering numerous potential applications. Our research group focuses on the discovery of new multiferroic materials within the perovskite family, with particular emphasis on naturally layered variants such as Ruddlesden-Popper and Dion-Jacobson (DJ) structures. The complexity of these materials, particularly those within the DJ family, presents challenges in understanding their structural pathways, which is essential to understand due to its correlation with polarization, typical of a highly ionic material. Conventional characterization techniques, like X-ray diffraction (XRD), often fall short in describing these systems transitions driven by rotations and tilts of oxygen octahedra. This limitation emphazises the need for alternative methods to study these materials effectively. In our study, we employ a local technique known as Perturbed Angular Correlation (PAC), which offers heightened sensitivity to quantum phenomena through the study of the electric field gradient (EFG), an essential property of the ground state. Furthermore, our investigation incorporates ab-initio simulations using Density Functional Theory (DFT). Focusing on CsNdNb2O7 [1,2] and CsLaNb2O7 DJ perovskites, we account for high quantum effects that influence this materials behavior. Our findings highlight the necessity of incorporating Hubbard corrections for specific atoms, such as Nd, to accurately describe the magnetic behavior and hyperfine parameters, thus contributing to a deeper understanding of these complex materials.

References
[1] Zhu T., et al., Chem. Materials 32, 10, 4340–4346 (2020).
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