

Abstract Submitted
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LDA+U Models of Polarons in LaBr₃ and CsI¹ JOHN JAFFE, SEBASTIEN KERISIT, KEVIN ROSSO, Pacific Northwest National Lab — We describe calculations of the formation and hopping energies of hole polarons (holes self-consistently localized in lattice distortions) in the wide-bandgap ionic materials LaBr₃ and CsI. Both one-center (breathing mode) and two center (anion dimer, also known as V_k center) polarons were treated. The LDA+U method based on the VASP code was employed, since standard DFT methods often fail to represent localized electronic states in solids. We used a 72-atom supercell of the UCl₃ structure for LaBr₃, and a 54-atom CsCl-structure unit cell for CsI. We attempt to correlate differences in electronic transport between these two compounds with different energy nonproportionality behavior that they exhibit as Ce-activated scintillators in gamma-ray spectroscopy.

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