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Small polarons and point defects in $LaFeO_3$ ZHEN ZHU, HARTWIN PEELAERS, CHRIS G. VAN DE WALLE, University of California, Santa Barbara — The proton-conductive perovskite-type $LaFeO_3$ is a promising negative-electrode material for Ni/metal-hydride (Ni-MH) batteries. It has a discharge capacity up to 530 $mAhg^{-1}$ at 333 K, which is significantly higher than commercialized AB_5-type alloys. To elucidate the underlying mechanism of this performance, we have investigated the structural and electronic properties of bulk $LaFeO_3$, as well as the effect of point defects, using hybrid density functional methods. $LaFeO_3$ is antiferromagnetic in the ground state with a band gap of 3.54 eV. Small hole and electron polarons can form through self- or point-defect-assisted trapping. We find that La vacancies and Sr substitutional on La sites are shallow acceptors with the induced holes trapped as small polarons, while O and Fe vacancies are deep defect centers. Hydrogen interstitials behave like shallow donors, with the donor electrons localized on nearby iron sites as electron polarons. With a large trapping energy, these polarons can act as electron or hole traps and affect the electrical performance of $LaFeO_3$ as the negative electrode for Ni-MH batteries. We acknowledge DOE for financial support.

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