Small polarons and point defects in LaFeO₃ ZHEN ZHU, HARTWIN PEELAERS, CHRIS G. VAN DE WALLE, University of California, Santa Barbara — The proton-conductive perovskite-type LaFeO₃ 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 AB₅-type alloys. To elucidate the underlying mechanism of this performance, we have investigated the structural and electronic properties of bulk LaFeO₃, as well as the effect of point defects, using hybrid density functional methods. LaFeO₃ 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 LaFeO₃ as the negative electrode for Ni-MH batteries. We acknowledge DOE for financial support.