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Modeling Correlation and Defect Effects on Mixed Polaronic and Ionic Transport in Rare-Earth Phosphates NICOLE ADELSTEIN, University of California at Berkeley — Rare-earth phosphates are promising candidates for intermediate-temperature proton-conducting fuel cell membranes, with Sr-doped $CePO_4$ showing particularly high conductivity in oxidizing conditions. Since this high conductivity is likely due to hole-polarons rather than protons, the defect chemistry of incorporating charge carriers (protons versus holes versus oxygen vacancies) is currently being investigated with experiments and calculations. In this work, the dominant charge carrier and its transport in $CePO_4$ is calculated with density functional theory and compared to conductivity and photon beam experiments. In particular, we present ab-intio calculations on the thermodynamics of the dopants and defects and proton and hole-polaron mobilities. For the case of hole-polaron mobilities, the strength of the coupling with the lattice and the electronic coupling between sites will be investigated.

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