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Hybrid Functional Calculations of Acceptor Doping in Protonic Conductor $SrZrO_3$ LEIGH WESTON, University of Sydney, ANDERSON JANOTTI, University of California, Santa Barbara, XIANGYUAN CUI, CATHERINE STAMPFL, University of Sydney, CHRIS VAN DE WALLE, University of California, Santa Barbara — Perovskite oxides such as $SrZrO_3$ (SZO), which exhibit high temperature proton conductivity, are promising electrolyte materials for use in solid oxide fuel cells (SOFCs). Proton conductivity in SZO is typically achieved via acceptor doping with trivalent cations substituting at the Zr site, where the formation of charge compensating oxygen vacancies facilitates proton solvation. We present a detailed study of Sc and Y dopants in SZO based on first-principles, hybrid density functional calculations. When substituting at the Zr site, both dopants form deep acceptors, where the neutral charge state forms a localized hole polaron state. Under certain growth conditions Sc and Y will form auto-compensating donor species by substituting at the Sr site, which would inhibit proton solubility. Moreover, the proton - dopant association was found to be strong, with proton binding energies of -0.41 eV and -0.31 eV for Sc_{Zr}^{-} and Y_{Zr}^{-} respectively, indicating that proton transport is limited by trapping. These new results will be useful in the development of zirconate based proton conducting electrolyte materials for solid oxide fuel cells.

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