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Small Polarons and Point Defects in Barium Cerate[1] MICHAEL SWIFT, ANDERSON JANOTTI, CHRIS G. VAN DE WALLE, Univ of California - Santa Barbara — Barium cerate ($BaCeO_3$) is a well-known proton-conducting material. In applications, it is frequently doped (for instance with yttrium) to increase stability and promote hydrogen uptake. However, the microscopic mechanisms of ionic conductivity and the effects of doping and native defects are still not fully understood. Many of the obstacles to the theoretical study of this material stem from the nature of the conduction band, which is made up of cerium $4f$ states. These states present a challenge to first-principles techniques based on density functional theory within the standard approximations for exchange and correlation. Using a hybrid functional, we investigate the effects of hydrogen impurities and native defects on the electrical and optical properties of $BaCeO_3$. We discuss the tendency of excess electrons or holes to localize in the form of small polarons. We also explore the interactions of polarons with hydrogen impurities and oxygen vacancies, and their impact on luminescence properties.

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