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Point defects and band alignment in strontium cerate[1] MICHAEL SWIFT, CHRIS G. VAN DE WALLE, Univ of California - Santa Barbara — Strontium cerate ($SrCeO_3$) is a well-known ionic conductor of both hydrogen and oxygen. In applications, it is frequently doped (for instance with yttrium or neodymium) to increase stability and promote diffusion. However, the microscopic effects of doping and native defects are not fully understood. Building on previous computational work in barium cerate ($BaCeO_3$), we use density functional theory with a hybrid functional to study impurities, electronic structure, and band alignments in these systems. We establish trends that we expect to hold across the perovskite cerates. We also discuss the alignment of the thermodynamic charge-state transition levels of hydrogen, and applications to this class of materials.

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