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**Hydrogen interstitials inside bulk reduced-$CeO_2$: charge state, defect chemistry and dynamics by *ab-initio* calculations**[1] LEI ZHANG, MEILIN LIU, Georgia Institute of Technology, MEILIN LIU TEAM — $CeO_2$ is a well-known and widely-used solid oxide fuel cells (SOFC) electrolyte and catalyst anode support, due to its facile oxygen vacancy formation and diffusion within its symmetric and capacious fluorite lattice. In real SOFC working conditions, hydrogen fuels will dissociate on anode surface and possibly permeate inside $CeO_2$-based anode support and electrolyte. Studying hydrogen defect inside $CeO_2$ lattice thus has two significant impacts: To see how hydrogen alters the "oxygen buffering" inside $CeO_2$ as an anode support, and to see how it affects oxygen vacancy's diffusion and clustering inside electrolyte $CeO_2$. Hereby *ab-initio* calculations in Kohn-Sham Density Functional Theory with Hubbard model of self-interaction correction is carried out to investigate the electron polaron and vacancy formation in $CeO_2$ affected by hydrogen, the hydrogen defect state within the band gap of $CeO_2$, the chemistry of defect interactions and its effect on oxygen vacancy mobility.

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