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A DFT+U study on oxygen-vacancy migration in rare-earth doped ceria: the role of 4f electrons. MUSA ALAYDRUS, Max Planck Inst fuer Eisenforschung GmbH, MAMORU SAKAUE, HIDEAKI KASAI, Osaka University — Development of novel fast ion conductors is a crucial issue for realizing solid oxide fuel cells (SOFCs), which can operate in low temperatures, below 600 ^{o}C. While yttria-stabilized zirconia (YSZ) had been well-studied both by experiments and theories, exploration of other types of materials retaining high ionic conductivities in lower temperatures is still desired. Here, we studied atomic and electronic properties of oxygen-ionic conduction of M-doped CeO2 based materials (M = La, Pr, Nd, Pm, Sm, Eu, Gd, and Y) by density functional theory (DFT) with Hubbard U correction in. The calculations were performed by considering two cases: (i) strongly localized 4f electrons, (i.e. f electrons are kept frozen in the core) and (ii) f electrons as valence electrons which requires many-body quantum mechanical treatments. The study suggests that balancing (meta-)stable energies can be considered as a key to optimize ionic mobility in doped CeO2. These energies are strongly associated with ionic/covalent interactions in the system. In the presentation we will show that fundamental aspects of the ionic/covalent interactions can only be explained in terms of variable occupancy of empty 4f orbitals.

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