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CeNbO₄ a potential electrolyte for solid oxide fuel cells MARTIN AMFT, NATALIA SKORODUMOVA, Uppsala University, DIVISION FOR MATERIALS THEORY TEAM — CeNbO₄ is a material of considerable interest for solid oxide fuel cells and other environmentally friendly applications. The low-temperature monoclinic phase of this material tends to be hyperstoichiometric incorporating extra oxygen up to CeNbO_{4.25}. Materials containing cerium are challenging to treat theoretically as strongly correlated materials are not well described by standard density functional theory. Here we study CeNbO₄ using the co-called LDA+U approach. We consider different interstitial positions for extra oxygen atoms and study how the formation energies of such defects depend on the degree of the localization of Ce f-states described by parameter U. We propose most likely interstitial sites for extra oxygen to occupy in the CeNbO₄ lattice and paths of oxygen migration.

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