Environment-dependent U for CeO_x from first principles

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DFT+U method has been widely used to describe localized electrons in strongly correlated materials, where a Hubbard U is introduced in the model Hamiltonian to account for the on-site screened Coulomb energy. In practice, the value of U is often obtained empirically by fitting to experimental data for reference systems, and may vary significantly depending the specific quantity used in the fitting. To reduce the degree of empiricism, in this work, we calculated U from *ab initio* theory using the linear response method (*Phys. Rev. B* **71**, 035105, 2005). Results for Ce oxides in different forms, e.g., crystal, surface and molecule, were analyzed, and trend that relates U to Ce valence states and the local chemical environment was discussed.

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