Abstract Submitted
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First-principles calculations of Ce activation in $RE_2M_2O_7$ (RE = La, Y; M = Ti, Zr, Hf).[1] ANURAG CHAUDHRY, ANDREW CANNING, ROSTYSLAV BOUTCHKO, STEPHEN DERENZO, NIELS GRONBECH-JENSEN — First-principles electronic structure calculations of Ce-doped La and Y compounds with composition RE2M2O7 (RE = La, Y; M = Ti, Zr, Hf) are performed using the pseudopotential method based on the local density approximation in density functional theory. The positions of the 4f states relative to the valence band maximum and the position of the lowest 5d excited state relative to the conduction band minimum of the host material are determined. The prediction of Ce activation is based on the following criteria: (1) The energy difference between the occupied Ce 5d excited state (Ce3+)* and the host material conduction band minimum (CBM) and (2) the degree of localization of the (Ce3+)* excited state on the Ce atom. Our theoretical investigations indicate that Ce activation is not possible in these host materials.

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