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Ab-initio calculation on electronic and optical properties of ThO_2, UO_2 and PuO_2

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Abstract

We have investigated the structural and electronic properties of oxides of Th, U and Pu using GGA+U method. Structure of these oxides is of cubic nature and they have indirect band gaps of 4.34 eV along M→R (ThO_2), 2.30 eV along Γ→R (UO_2) and 2.27 eV along M→R (PuO_2). The density of states (DOS) of these oxides shows main contribution of 2p orbital in valence band maxima of ThO_2 and PuO_2 while in UO_2 5f orbital contributes mainly in VBM. We also investigated the optical properties of these oxides and found that static dielectric function increases from ThO_2 to PuO_2.

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