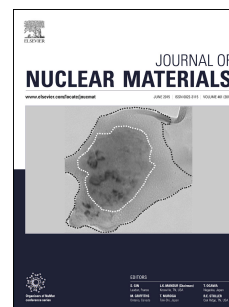


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Ab-initio calculation on electronic and optical properties of ThO₂, UO₂ and PuO₂

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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 (ThO₂), 2.30 eV along Γ →R (UO₂) and 2.27 eV along M→R (PuO₂). The density of states (DOS) of these oxides shows main contribution of 2p orbital in valence band maxima of ThO₂ and PuO₂ while in UO₂ 5f orbital contributes mainly in VBM. We also investigated the optical properties of these oxides and found that static dielectric function increases from ThO₂ to PuO₂.

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Keywords: Electronic band structure, Partial density of states, density functional theory, optical properties

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