First-principles calculations of physical properties of light actinide oxides.

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We present a first-principles study of light actinide oxides. By performing density functional theory calculations with the GGA+*U* method, we have calculated the structural stability and magnetic property of the higher than tetravalent oxidized compounds, namely U_3O_8 and Np_2O_5. From the calculated electronic structure, the U or Np 5*f* - O 2*p* hybridization has been analyzed. Also, we have investigated the chemical reactivity of Pu atoms in PuO_2 and compared the electron density of states of it for different oxidation states of Pu with experimental data for X-ray spectra. In order to understand lattice dynamics of actinide oxides, we have performed phonon calculations for ThO_2, UO_2, and PuO_2 and compared the phonon dispersion curves with each other. q