

4f-Heprul Córepil

111: 121254e The 4f binding-energy shifts of the light-actinide dioxides and tetrafluorides. Cox, L. E.; Farr, J. D. (Mater. Sci. Technol. Div., Los Alamos Natl. Lab., Los Alamos, NM 87545 USA). Phys. Rev. B: Condens. Matter 1989, 39(15), 11142-5 (Eng). The 4f binding energies of NpF4 and PuF4 were measured, and are discussed in terms of those of the oxides and fluorides of the light actinides. Although the electronegativities of these elements are nearly const., the chem. shifts for each series show a regular increase relative to the metals. From results of previously reported band-structure and mol.-orbital calcus., the shifts are shown to result from increasing differences in 5f occupation and, to a lesser extent, increase in the 5f-core-level Coulombic interaction. Recently reported L₃ x-ray-absorption and renormalized-atom calcus. are used to assess the importance of final-state screening energies in both the metals and the insulating compds.

® Pufy ○ c.A. 1989, 111, N14

[99] Mp Fy Carnall W.T., Liu G.K. et al. J. Chem. Phess. 1991. 98, N 10.C. 4194-4203 ulf.n. (ell. UFy; III)