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Phase stability of actinide carbides

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Electronic, structural, mechanical, magnetic and thermodynamical properties of uranium and thorium sesquicarbides (U_2C_3 and Th_2C_3) were investigated by the means of first principles calculations, with special interest in the effects of $5f$ electrons. Utilized models included various approximations of exchange-correlation electronic terms, spin-orbital interaction (with a major effect on U_2C_3 and egligible effect on Th_2C_3) and Hubbard U model for electronic Coulomb interaction. The magnitude of these effects is demonstrated on the direct comparison of various physical quantities, such as band structure, enthalpy of formation, magnetic ordering, heat capacity, elastic constants, etc. and compared with experimental data.

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