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Rotational Rehybridization and the High Temperature Phase of UC₂

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Abstract

The screened hybrid approximation (HSE) of density functional theory (DFT) is used to examine the structural, optical, and electronic properties of the high temperature phase, cubic UC₂. This phase contains C-2 units with a computed C-C distance of 1.443 angstrom which is in the range of a CC double bond; U is formally 4+, C-2 4-. The closed shell paramagnetic state (NM) was found to lie lowest. Cubic UC₂ is found to be a semiconductor with a narrow gap, 0.4 eV. Interestingly, the C-2 units connecting two uranium sites can rotate freely up to an angle of 30 degrees, indicating a hindered rotational solid. Ab-initio molecular dynamic simulations (HSE) show that the rotation of C-2 units in the low temperature phase (tetragonal UC₂) occurs above 2000 K, in good agreement with experiment. The computed energy barrier for the phase transition from tetragonal UC₂ to cubic UC₂ is around 1.30 eV per UC₂. What is fascinating about this system is that at high temperature, the phase transformation to the cubic phase is associated with a rehybridization of the C atoms from sp to sp(3).

Keywords

KeyWords Plus: [DENSITY-FUNCTIONAL THEORY](#); [TETRAGONAL TRANSFORMATION](#); [MOLECULAR-DYNAMICS](#); [PHOTOEMISSION](#); [DICARBIDES](#); [CARBIDES](#); [URANIUM](#); [METALS](#)

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