Importance of the electron correlations and spin-orbit coupling for lattice dynamics of UC

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Uranium monocarbide, a potential fuel material for the generation IV reactors, is investigated within density functional theory. Its electronic, magnetic, elastic, and phonon properties are analyzed and discussed in terms of spin-orbit interaction and localized versus itinerant behavior of the $5f$ electrons. The localization of the 5f states is tuned by varying the local Coulomb repulsion interaction parameter. We demonstrate that the theoretical electronic structure, elastic constants, phonon dispersions, and their densities of states can reproduce accurately the results of x-ray photoemission and bremsstrahlung isochromat measurements as well as inelastic neutron scattering experiments only when the $5f$ states experience the spin-orbit interaction and simultaneously remain partially localized. The partial localization of the $5f$ electrons could be represented by a moderate value of the on-site Coulomb interaction parameter of about 2 eV. The results of the pres ent studies indicate that both strong electron correlations and spin-orbit effects are crucial for realistic theoretical description of the ground-state properties of uranium carbide. [1] We compare the novel material to the at presence used most common nuclear fuel material, UO_2 oxide. Here are calculations show that considering the exchange and electron correlations effects the generalized gradient approximations was succesfully in descrption of the phonon dispersion spectrum, thermal expansion, and heat capacity w.r.t to the recorded data.[2] For both materials the so-called direct method, based on the quasiharmonic approximation, was used. To study the pressure dependence of the phonon frequencies of UO_2 we calculate phonon dispersions for several lattice constants. Our computed phonon spectra demonstrate the opening of a gap between the optical and acoustic modes induced by pressure. Taking into account the phonon contribution to the total free energy of UO_2 it s thermal expansion coefficient and heat capacity have been computed from first-principles. Both quantities are in good agreement with available experimental data for temperatures up to about 500 K.

[1] U.D. Wdowik et al., *Phys. Rev. B* **94**, 054303 (2016).
[2] Y. Yun et al. , *J. Nucl. Mater.* **426**, 109 (2012).