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Crystal field and magnetic structure of UO_2: a computational probe of the multi-determinantal ground and excited states[1] FEI ZHOU, UCLA, VIDVUDS OZOLINS — The properties of UO_2 is the result of complex f-electron physics, characterized by localization of orbitals, strong electronic interactions and spin-orbit effects, crystal field potential, magnetic and electron-lattice couplings. We present a comprehensive theoretical study of the electronic structure of UO_2 with combined applications of a newly improved density functional method and a model Hamiltonian. The model, unambiguously parametrized with DFT calculations, predict the excitation energies of the f^2 states, including the whole spectrum with different L, S, J as well as the low energy crystal field excitations $\Gamma_5 \rightarrow \Gamma_{3,4,1}$, with good agreement to experiment. The Γ_5 triplet is confirmed as the lowest multiplet. We also investigated different non-collinear magnetic structures, in particular the 3-k ground state, of UO_2.

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