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Effects of full Coulomb interactions on electronic structure of δ-Pu EUGENY GORELOV, TIM WEHLING, HARTMUT HAFFERMAN, ALEXANDER LICHTENSTEIN, University of Hamburg, ALEXEY RUBTSOV, Moscow State University, ALEXANDER LANDA, CHRIS MARIANETTI, MICHAEL FLUSS, Lawrence Livermore National Laboratory, ALEXEY SHORIKOV, ALEXEY LUKOYANOV, MICHAEL KOROTIN, VLADIMIR ANISIMOV, Institute of Metal Physics — We used the CTQMC method for the realistic simulation of electronic properties of correlated actinides. In particular, we focus on the spectral function of δ-Pu, which is described in terms of a 7-orbital f-impurity model interacting with a metallic bath. Our CTQMC implementation solves this model by calculating a weak coupling expansion of the partition function in the fermionic multiorbital path-integral representation and provides numerically exact results for relatively high temperature. We discussed how different terms in the full on-site Coulomb vertex affect the local density of states. The comparison of CTQMC results with only diagonal density-density like Coulomb interactions and with additional non-diagonal terms in the interaction part of the Hamiltonian related with so-called spin flips terms shows the importance of the full rotationally invariant Coulomb vertex on the electronic structure of δ-Pu. This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

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