Electronic Correlation Effects in Plutonium Metals and Compounds

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An understanding of the phase diagram of elemental plutonium (Pu) must include both the effects of the strong directional bonding and the high density of states of the Pu 5*f* electrons, as well as how that bonding weakens under the influence of strong electronic correlations. In this talk, I will give an LDA+DMFT perspective on the electronic correlation effects in Pu elemental solids and compounds. After a brief overview of the earlier results of electronic structure calculations on the δ-phase of Pu, I will discuss the Kondo physics of Pu impurity in a non-interacting bath [1], and then proceed to discuss the electronic structure of the true α-phase of Pu [2] and Pu-115 compounds [3]. A further development of the DMFT-based first-principles approach will be briefly discussed.

[1] Jian-Xin Zhu, R. C. Albers, K. Haule, and J. M. Wills, Phys. Rev. B **91**, 165126 (2015).

[2] Site-selective electronic correlation in a-plutonium metal, Jian-Xin Zhu, R. C. Albers, K. Haule, G. Kotliar, and J. M. Wills, Nat. Commun. **4**, 2644 (2013).

[3] Jian-Xin Zhu et al. (to be published).