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Combined LDA+Exact Diagonalization Study for Actinide Compounds ALEXEY GORDIENKO, SERGEY SAVRASOV, University of California, Davis — Exact diagonalization (ED) is a most straightforward and powerful way to study problems related to strong electron correlations, but very computationally demanding for f-electron systems. Computational efficiency of the ED approach can be greatly increased with help of iterative methods and we shall present our recent ED implementation which makes use of Kernel Polynomial Method (KPM) to calculate temperature Green's Function and self-energy. This allows us to deal relatively easy with problems whose size is $5{\cdot}10^5$ states that is a characteristic for impurity problems with f-electrons. As an application, actinide compounds PuO_2 and UO_2, will be studied self-consistently using self- energies extracted from cluster ED and combined with electronic structure LDA calculation.

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