Importance of correlations effects, spin-orbit coupling in heavy elements vs. actinides using Density Functional Theory approach

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Thermal expansion and thermal conductivity are the key properties for nuclear reactor fuel design. This considers the actinides and actinide compounds mainly. Those are formed from heavy elements and its physics of complex behavior of the 5f electronic shell. In this lecture we learn how to treat relativistic effects using quantum-mechanical calculations and lattice dynamics (atomic vibrations) in order to determine thermal expansion and thermal conductivity, i.e the electron as well as phonon contributions to these quantities. Success of the approach depends how accurate one can determinate the electronic structure of given system with respect to the physical quantity (phenomena) of interest, here often complicated by the physics of itinerant vs. localized behavior of the 5f shell. Here we tackle the effects of electron correlations as well as the effect of the the role of relativistic effects (e.g. spin-orbit coupling) and determine to which extent and for which material they play a decesive role for such usefull and measureable quantities like thermal expansion and thermal conductivity. More details and for the future reference of the described phenomena could be found in Ref. [1-5].

References:

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