Thoria Notes

Murphy does point defects in ThO2[1].

The DFT calculations described here were performed using the frozen-core all-electron projector-augmented-wave PAW method[2, 3], as implemented in the *ab-initio* total energy code VASP (Vienna *ab-initio* simulation program).

UO2

Defects in UO2

Dorado +U corrections for UO2[4]

1. Murphy, S., M. Cooper, and R. Grimes, *Point defects and non-stoichiometry in thoria.* Solid State Ionics, 2014. **267**: p. 80-87.

2. Blöchl, P.E., *Projector augmented-wave method.* Physical Review B, 1994. **50**(24): p. 17953.

3. Kresse, G. and J. Furthmüller, *Efficient iterative schemes for ab initio total-energy calculations using a plane-wave basis set.* Physical Review B, 1996. **54**(16): p. 11169.

4. Dorado, B., et al., *Advances in first-principles modelling of point defects in UO2: f electron correlations and the issue of local energy? minima.* Journal of Physics: Condensed Matter, 2013. **25**(33): p. 333201.