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First principles LDA + U and GGA + U study of protactinium and protactinium oxides: Dependence on the effective U parameter

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Abstract content
   (Max 300 words)

The electronic structure and properties of Protactinium and its oxides (PaO and PaO2) have being studied in the frame work of the LDA, GGA(PBE), LDA+U and GGA(PBE)+U implementations of density functional theory. The dependence of selected observables of these materials on the effective U parameter has being investigated in detail. The examined properties include lattice constants, bulk modulus, effect of charge density distribution, hybridisation of the 5f orbital and energy of formation for PaO and PaO2. The LDA+U gives a better agreement with experiment than the GGA+U for the structural properties of Pa. We obtained that PaO is metallic and PaO2 is an mott-hubbard insulator within the DFT+U approximation. This is consistent with observations for other actinide oxides, unlike GGA and LDA which gives metallic behaviour for PaO2. The calculated band gap reported for PaO2 is a prediction and should stimulate further studies.

Apply to be
 consider for a student
   award (Yes / No)?

Yes

Level for award
 (Hons, MSc,
   PhD)?

PhD

Main supervisor (name and email)
and his / her institution

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Would you like to
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No

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