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Electronic and mechanical properties of the actinide mononitride and dinitride

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Abstract content
   (Max 300 words)

We present a detailed comparative study of the electronic and mechanical properties of the actinide mononitrides and actinide dinitrides within the frame work of the Perdew-Burke-Ernzerhof generalized gradient approxima- tion (GGA [PBE]) and GGA + U implementations of density functional theory with the inclusion of spin-orbit coupling. The dependence of selected observables of these materials on the effective U-parameter has been investigated in detail. The examined properties include the lattice constants, bulk modulus, effect of charge density distribution, hybridization of the 5f orbital and energy of formation for actinide nitride compounds. The Hubbard U parameter is included to give a proper description of the 5f electrons, and subsequently accurately determine the structural and electronic properties of the compounds. The mononitride and dinitride of all the actinide nitrides investigated using GGA (PBE) and GGA [PBE] + U approach is metallic except UN2 which is an insulator. Also UN, NpN, PuN, NpN2 and PuN2 are magnetic systems with an orbital dependent magnetic moments oriented in the z-axis.

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Yes

Level for award
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PhD

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

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