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Physical Properties of Uranium Dinitride UN2 by Using Density Functional Theory (DFT and DFT+U)

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Abstract : Physical properties of uranium di-nitride (UN2) were investigated in detail using first principles calculations based on density functional theory. To treat the strong correlation effects caused by 5f Uranium valence electrons, on-site Coulomb interaction correction via the Hubbard-like term, U (DFT+U) was employed. The UN2 structural, mechanical and thermodynamic properties were calculated within DFT and Various U of DFT+U approach. The Perdew–Burke–Ernzerhof (PBE.5.2) version of the generalized gradient approximation (GGA) is used to describe the exchange-correlation with the projector-augmented wave (PAW) pseudo potentials. A comparative study shows that results are improved by using the Hubbard formalism for a certain U value correction like the structural parameter. For some physical properties the variation versus Hubbard U is strong like Young modulus but for others it is weakly noticeable such as the density of state (DOS) or bulk modulus. We noticed also that up from U=7.5 eV, elastic results become not conform to the cubic cell elastic criteria since the C44 values turn out to be negative.

Keywords : uranium diNitride, UN2, DFT+U, elastic properties
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