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DFT studies of the effect of magnetic ordering and Hubbard U on the properties of UN

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Metallic ceramic fuels, for example, UN, are very interesting materials as their thermal conductivity remains high even at very high temperatures due to significant electronic heat transport. They are important because urania fuel, which is used in conventional nuclear reactors, is not the optimum option for some designs of new-generation reactors due to its low thermal conductivity. U-density (34.2 atoms/nm3) in UN is higher than in UO2 (24.47 atoms/nm3); therefore, it is more economical and suitable for implementation as a lower enrichment (LEU) fuel.

We have investigated the effect of magnetic ordering and Hubbard U (HU) on electronic transport and elastic properties of UN using first-principles methods. The generalized gradient approximation (GGA) of the Perdew, Burke, and Hubbard U, implemented in VASP code, and the new BoltzTrap2 code were used. Although we found that the free energy is lower for ferromagnetic ordering than non-magnetic or antiferromagnetic state, only antiferromagnetic ordering with GGA + HU = 3.5 eV predicted the electronic transport of UN in agreement with the experiment.

Keyword-1

Density Functional Theory

Keyword-2

Electronic transport

Keyword-3

Magnetic ordering

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