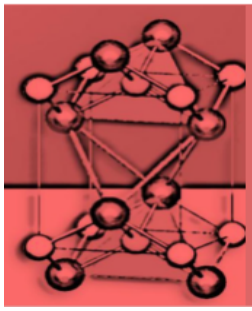

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Dependence of the formation energy with the Kohn-Sham solution method and exchange-correlation functional for the XN (X=Al, Ga, In) semiconductors

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Theoretical and computational studies of materials through Density Functional Theory (DFT) are widely used in solid-state physics to characterize, describe, and predict the properties of diverse and new compounds. One of the parameters to consider is the formation energy of the compound, which gives an idea of its energetic stability. In this study, the formation energies (Ef) of the binary AlN, GaN, and InN semiconductors are reported, and its dependence on the method used to solve the self-consistent Kohn-Sham equations is investigated. The methods used are the Full Potential Augmented Plane Wave (FP-LAPW) method, implemented in the Wien2k code, and the Pseudopotential and Plane Wave (PP-PW) method, implemented in the Quantum Espresso code.
For the PP-PW method, NormConserving, Ultrasoft, and PAW type pseudopotentials are considered. In addition, the dependence of Ef on the exchange-correlation part (XC) is analyzed, where the Local Density Approximation (LDA) is considered with the PW91 parametrization, and the Generalized Gradient Approximation (GGA) with the parametrizations PBE, PBEsol, and WC.
The results show that the formation energies of AlN, GaN, and InN are found to be sensitive to both, the method used to solve the Kohn-Sham's equations, and the XC functional.