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Strain and crystal field splitting inversion in III-Nitrides

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The wurtzite phase group III-Nitrides (AlN, GaN, InN) have attracted great interest due to their successful applications in the optoelectronics since the 90's. In this paper we perform a comprehensive study of AlN, GaN and InN structural elastic and electronic properties using hybrid and conventional Density Functional Theory, presenting a comparison of the features of the three compounds. We perform a direct comparison of the features of their electronic structures, including the inversion of the top valence band associated with a negative crystal field splitting and its relation to the challenges of acceptor-doping on AlN systems. With the determination of elastic constants and the Young modulus we provide a simple model to connect a deformation energy associated with the parameter u and the effective crystal-field splitting, showing a direct relation among internal strain and the crystal-field splitting.

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