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A Hybrid Look at Band Offsets in AlN/GaN Heterostructures
JEREMY NICKLAS, JOHN WILKINS — Hybrid functionals have been gaining traction for their better estimation of band gaps in semiconductors. Recently, a screened hybrid functional, HSE, has been introduced that improves upon the hybrid functionals by essentially screening out the Fock exchange after a given radius. This study compares how well the HSE functional does with the technologically important band offsets in the AlN and GaN wide bandgap heterostructures compared to experiment and other previous theoretical calcuations. Both the strained polar hexagonal and the nonpolar cubic phases of these III-V semiconductors are taken into consideration. Due to the large induced electric field in the polar hexagonal strucuture, a multipole decomposition will be discussed as well.

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