# Investigation of energetics of nitride systems based on self-consistent hybrid functional

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As exemplified from the III-V semiconductors like GaN, nitride materials are widely applied for the optoelectronic applications. Besides of such light emitting devices, recently, nitrides are also receiving attentions as a candidate for high-performing photovoltaic materials due to their high tolerance against defect and superior carrier transport, etc[1]. To design and screen nitride materials for the optoelectronic and photovoltaic applications, an accurate understanding of nitride electronic structure is thus critically required. However, current density functional theory (DFT) based on semi-local approximations suffers from the well-known bandgap underestimation problem originated from the self-interaction error. In this work, we employ the self-consistent hybrid functional method developed by J. H. Skone, et al.[2] to investigate the electronic structures of 13 different nitrides. By self-consistently determining the dielectric constant and the Hartree-Fock exchange ratio of the hybrid functional, we obtain accurate bandgap properties for nitrides comparable to the previous GW calculation results. We further investigate the band alignments of various nitrides, which can be used as a guideline for the design of nitride-based photophysical systems.

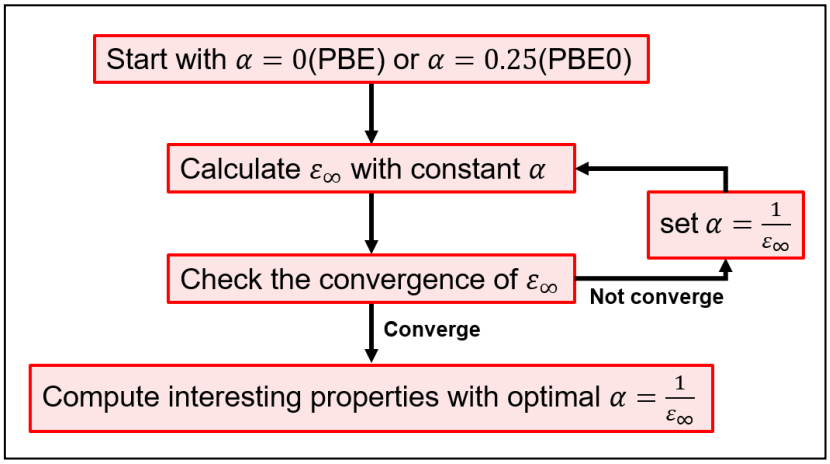


**Figure 1 Self-consistent iteration scheme for determining $\alpha = 1/\varepsilon_\infty$**

**References**

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[2] J. H. Skone *et al*., "Self-consistent hybrid functional for condensed systems," *Physical Review B*, **89**, 195112-195123 (2014).