

Cite this: DOI: 10.1039/xxxxxxxxxx

Supplemental material: Dimension-dependent band alignment and excitonic effects in graphitic carbon nitride: a many-body perturbation and time-dependent density functional theory study

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Received Date
Accepted Date

DOI: 10.1039/xxxxxxxxxx

www.rsc.org/journalname

1 Density of States

The calculated total and partial density of states (DOS) of g-h-triazine C₃N₄ is shown in figure 1.

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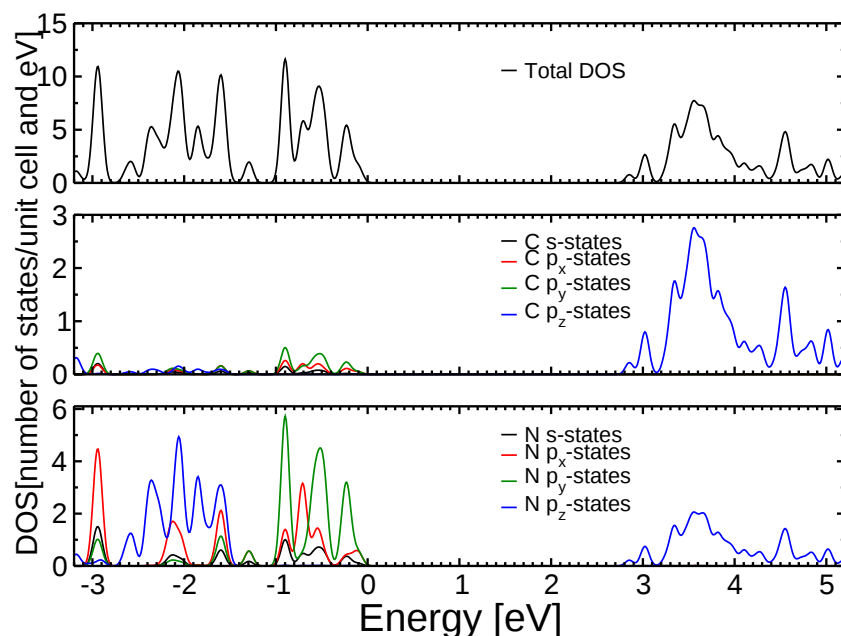


Fig. 1 Calculated total and partial DOS by optB88+G₀W₀ for bulk g-C₃N₄. A Gaussian broadening with a FWHM = 0.1 eV was used to smear out the calculated DOS.