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XAS, XES and DFT simulations to bridge local and macroscopic properties in GaAsN

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Although it is well known that dilute species often significantly modify the properties of solids in which they are hosted, a basic question remains open: how critical are their local properties in determining the macroscopic ones of the host material? Here, we address this issue by taking N in dilute III-V-N alloys as a paradigmatic case and propose an original approach based on synergic use of x-ray spectroscopies (XANES and valence – to – core XES at the N K-edge), density functional theory simulations and hydrogen exposure as a tool to modify N local bonding. Our results disclose the key role of the local N – Ga interactions in determining both N-related band states and the macroscopic effects of dilute N on the GaAs energy gap. The success of our approach indicates a new way to connect local and macroscopic properties.

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