nanomaterials

MDPI

# Supplement Materials: Investigation on structure-property relationships of 2D Ga/In chalcogenides

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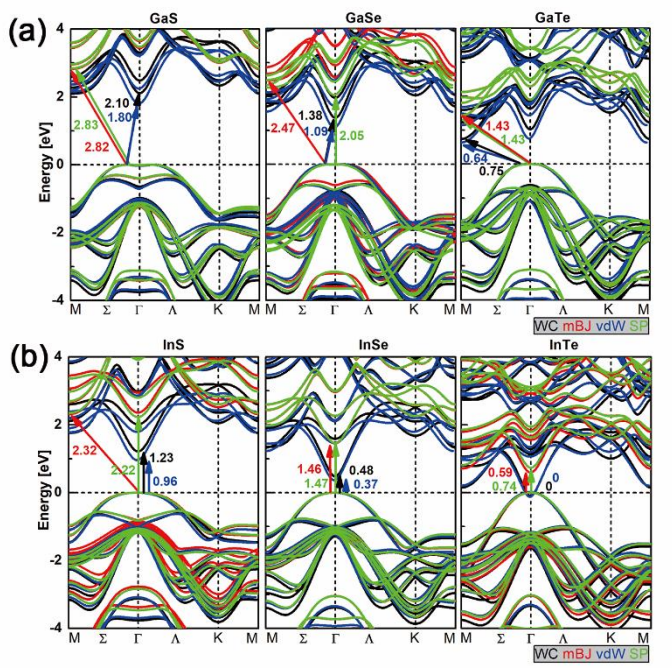


**Figure S1.** Band structures of bulk GaX **(a)** and InX **(b)** (X=S, Se, Te) calculated using WC-GGA with (green curves) and without polarization (black curves), mBJ (red curves) and optB88-vdW (blue curves) functionals.

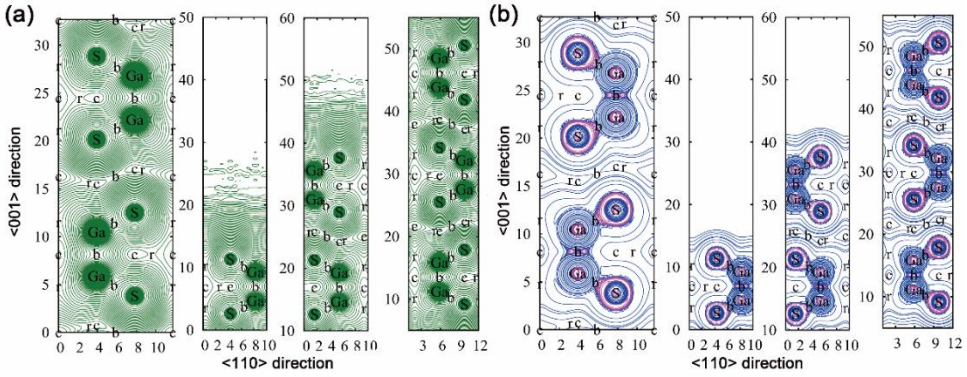


**Figure S2.** Electron density **(a)** and Laplacian **(b)** distributions of bulk, mono-, bi, and trilayered GaS in (-110) plane. Labels "b", "r" and "c" represent bond, ring and cage critical points at the zero-flux surface respectively.

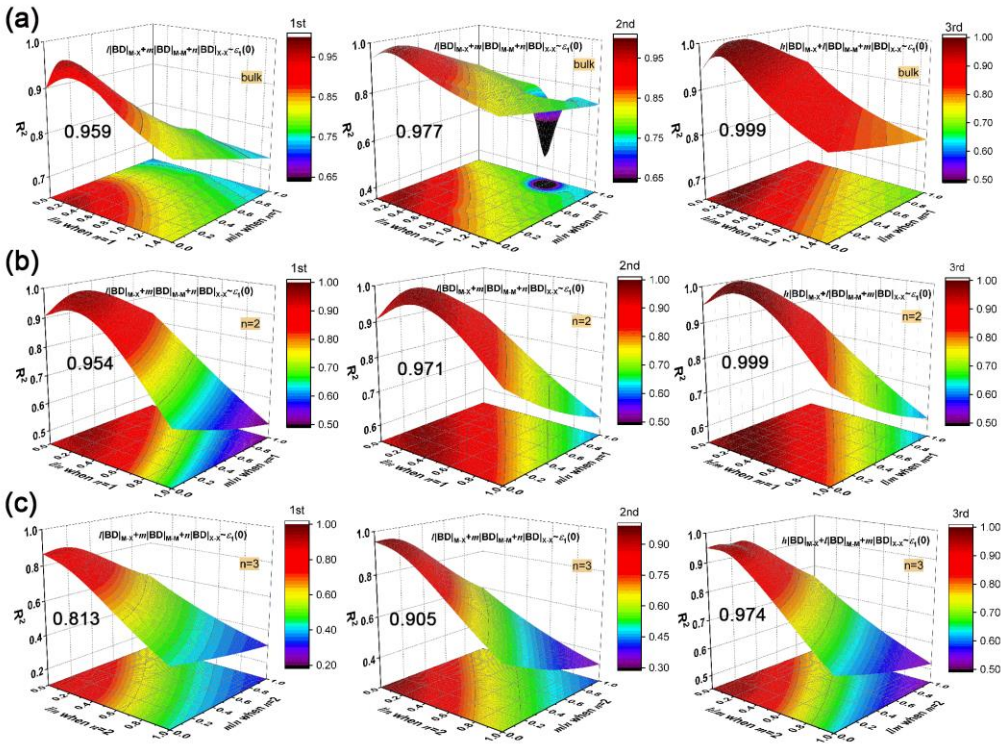


**Figure S3.** Polynomial fitting $h|BD|_{M\text{-}X}+l|BD|_{M\text{-}M}+m|BD|_{X\text{-}X}$ vs. $\varepsilon_1(0)$ as equation order goes from the first to second and to third: Coefficient of determination $R^2$ of bulk **(a)**, bilayer **(b)**, trilayer **(c)** by adjusting $h/m$ and $l/m$ ratios and their respective maximum $R^2$.

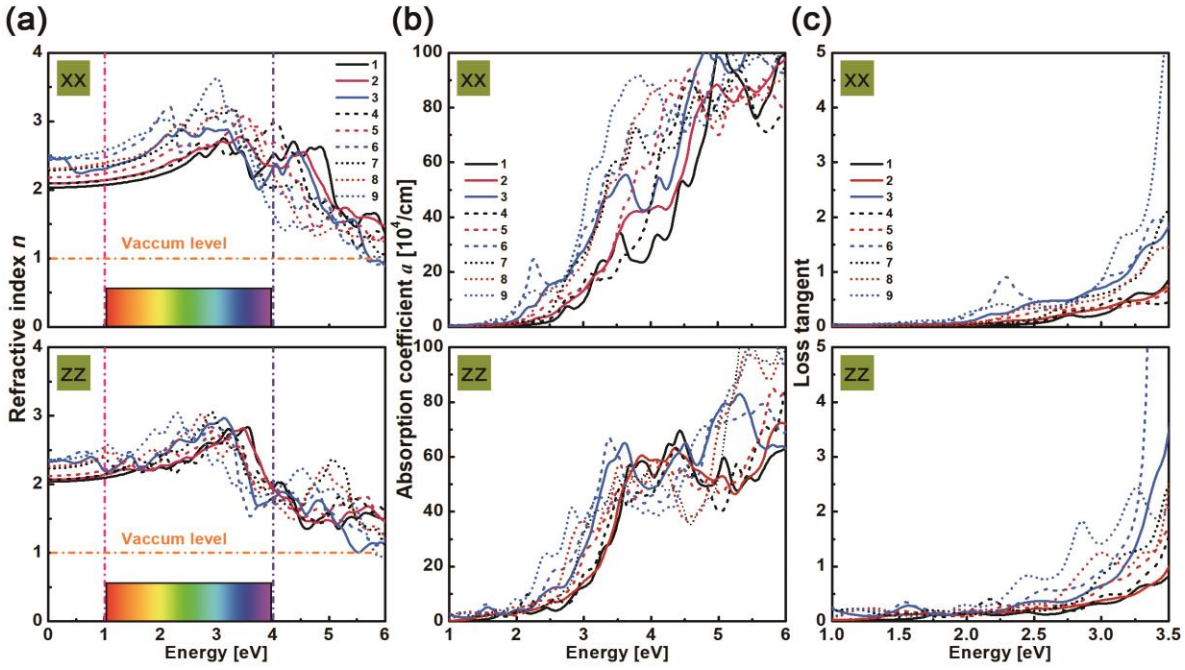


**Figure S4.** In-plane ($xx$) and out-of-plane ($zz$) refractive indexes **(a)**, absorption coefficients **(b)** and loss tangents **(c)** of N°1-9 GaX/InX.

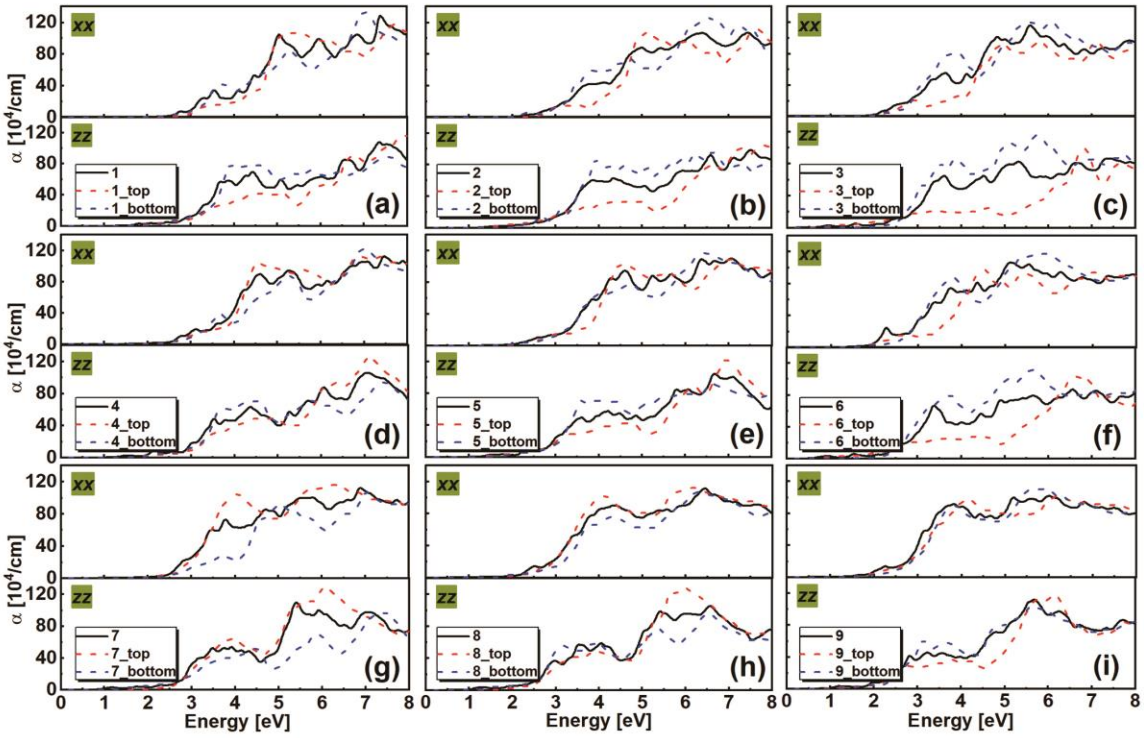


**Figure S5.** In-plane (*xx*) and out-of-plane (*zz*) absorption coefficients of N°1-9 GaX/InX compared with those of their constitutive top and bottom bilayers **(a)-(i)**.

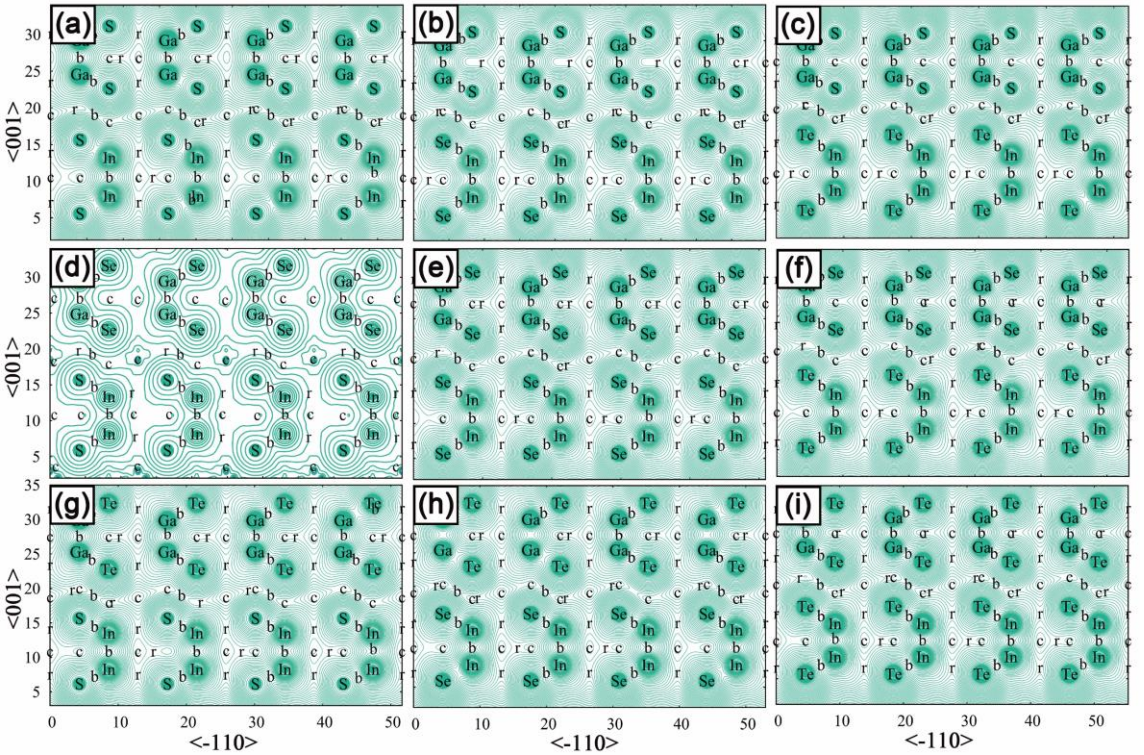


**Figure S6.** Electron density distributions of N°1-9 GaX/InX along the <110> plane **(a)-(i)**. Labels "b", "r" and "c" represent bond, ring and cage critical points at zero-flux surface respectively.

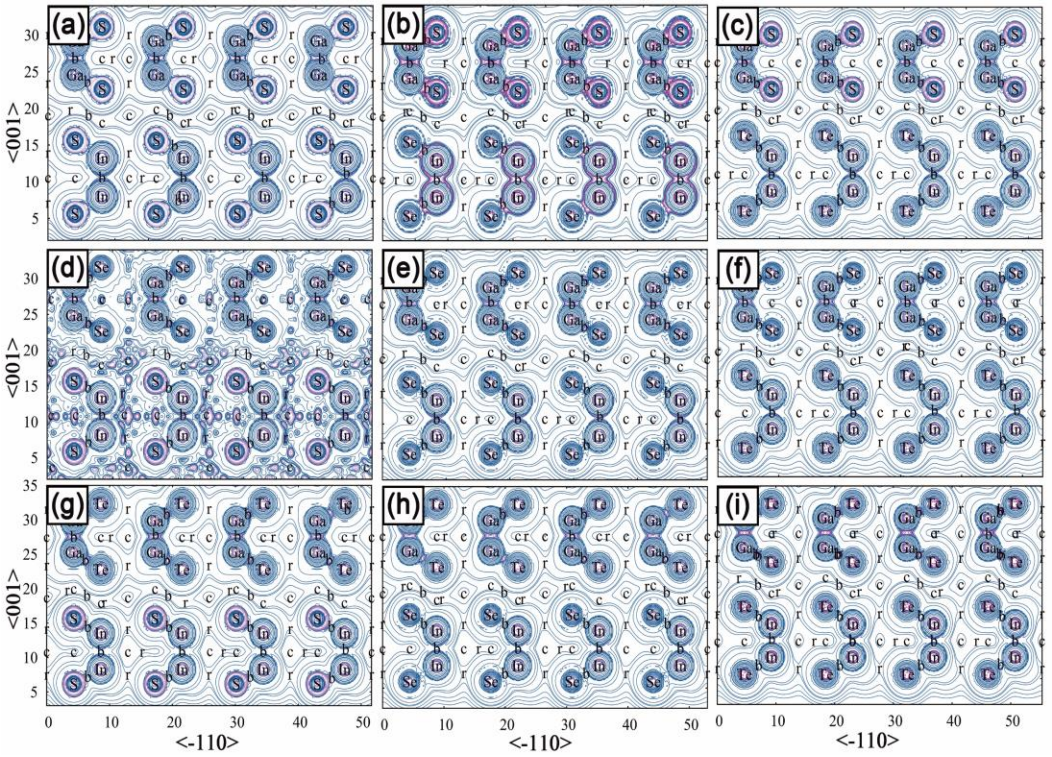


**Figure S7.** Laplacian of electron density distributions of N°1-9 GaX/InX along the <110> plane **(a)-(i)**. Labels "b", "r" and "c" represent bond, ring and cage critical points at zero-flux surface respectively.

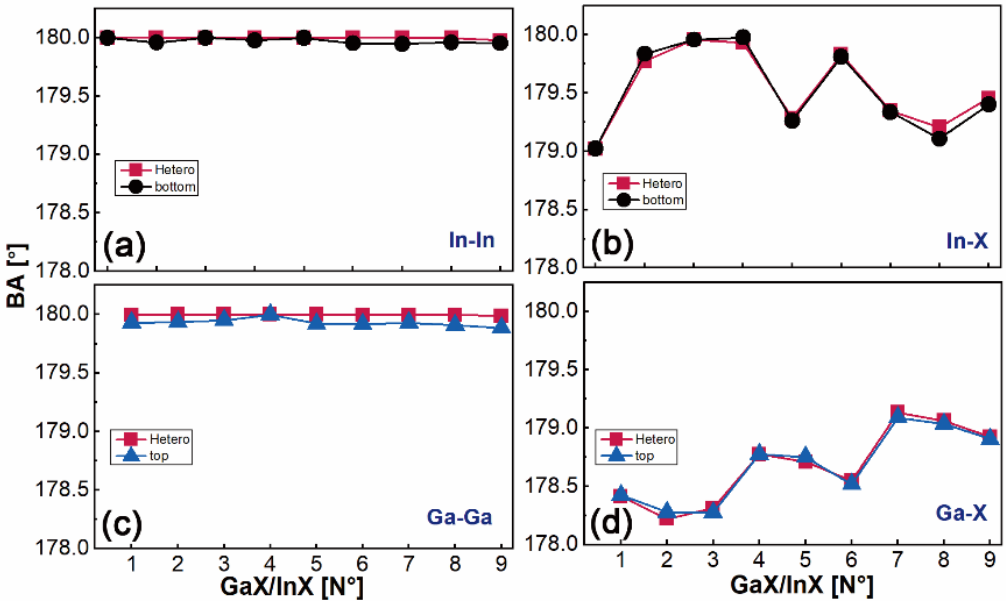


**Figure S8.** Bond angle (BAs) of In-In **(a)**, In-X **(b)**, Ga-Ga **(c)** and Ga-X **(d)** bonds of N°1-9 GaX/InX (red color), and the constitutive top $[GaX]_2$ (blue color) and bottom $[InX]_2$ (black color).