Supplementary material for: Native defects in monolayer GaS and GaSe: electrical properties and thermodynamic stability

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I. CALCULATION OF DIELECTRIC CONSTANTS

Static dielectric constants were calculated applying the method presented in Ref. [1] to $a \times a \times na$ (n = 2, 4, 8, 16) supercells, with a being the in-plane lattice constants. As an example, in Fig. 1 we show the PBE-D results as obtained directly from the supercell calculations and from applying the correction proposed by Noh et al. [1]. The values presented in Table I in the main body of the paper reflect the converged and corrected constants, Figs. 1(b) and 1(d).

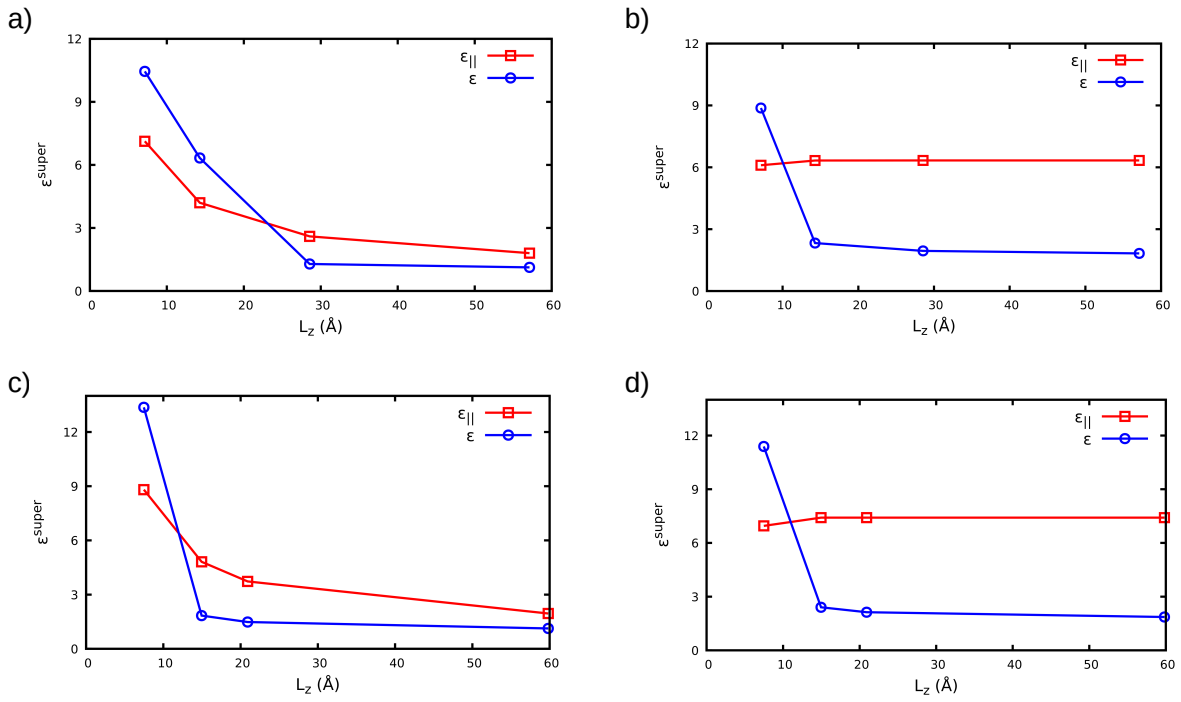

FIG. 1. PBE-D calculated in-plane ($\varepsilon_{\parallel}$) and out-of-plane ($\varepsilon_{\perp}$) components of the dielectric constants of monolayer GaS and GaSe. On the one hand, (a) and (c) show the corresponding values as directly obtained from supercell calculations. On the other hand, (b) and (d) present the corrected values as obtained using the method proposed in Ref. [1].

II. RELAXED DEFECTS STRUCTURES FOR GALLIUM SELENIDE

As done for GaS in the main body of the paper, in Fig. 2 we present the relaxed geometries of the studied native defects in monolayer GaS and in their charge neutral state.

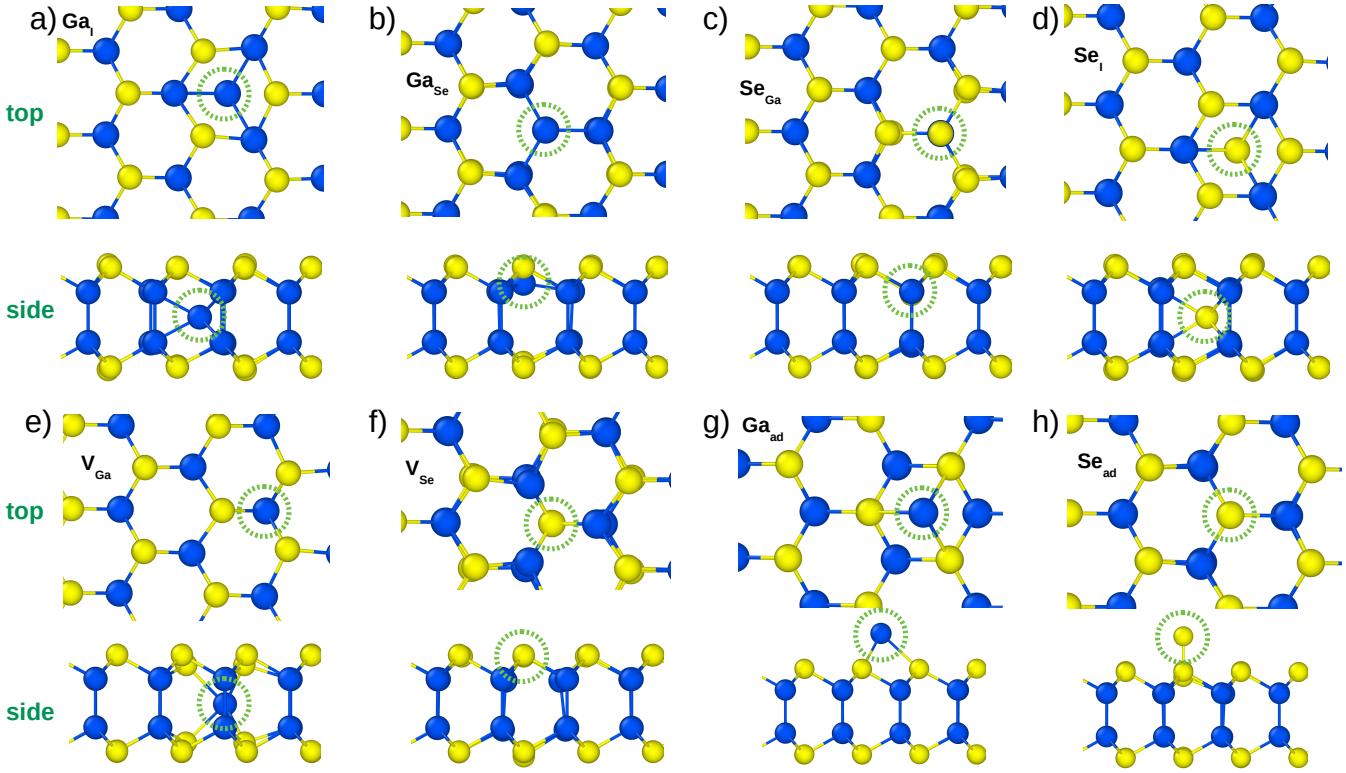

FIG. 2. Relaxed structures of native defects in monolayer GaSe in their neutral charge state, as obtained from PBE-D calculations. (a) Ga_i, (b) Ga_{Se}, (c) Se_{Ga}, (d) Se_i, (e) V_{Ga}, (f) V_{Se}, (g) Ga_{ad}, (h) Se_{ad}. For each case top and side views are shown, and green circles mark the position of the defects. Ga and Se atoms are shown in blue and yellow, respectively. Results using the HSE06 functional only show negligible differences with respect to the structures shown here. Visualization of the structures is done with OVITO [2].

[1] J.-Y. Noh, H. Kim, and Y.-S. Kim, Phys. Rev. B **89**, 205417 (2014).

[2] A. Stukowski, Modelling and Simul. Mater. Sci. Eng. **18**, 015012 (2010).