

Supplementary Information for

Hybrid functional calculation of electronic and thermoelectric properties of GaS, GaSe, and GaTe monolayer

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Energy minimization

The total energy as a function of lattice constant for GaS, GaSe, and GaTe monolayers are calculated as shown in Fig. S1. It is found that GaS, GaSe and GaTe monolayer have lowest energy at 3.636 Å, 3.814 Å and 4.140 Å respectively.

Effective mass

The effective mass (m^*) of an electron (hole) in a semiconductor with a given (E, k) value is given by

$$\left(\frac{1}{m^*}\right)_{ij} = \frac{1}{\hbar^2} \frac{\partial^2 E(k)}{\partial k_i \partial k_j} \quad (S1)$$

where i and j are Cartesian coordinate.

$$E(k) = ak^2 + bk + c$$

$$\frac{d^2 E}{dk^2} = 2a$$

The effective mass were evaluated by the inverse of second derivative of $E(k)$ with respect to k :

$$m^* = -\frac{\hbar^2}{2a} \quad (S2)$$

The fitting of quadratic equation to the valence band maximum (VBM) and conduction band minimum (CBM) of the GaS, GaSe and GaTe monolayer along either side of k -point are shown in Fig. S2-S7.

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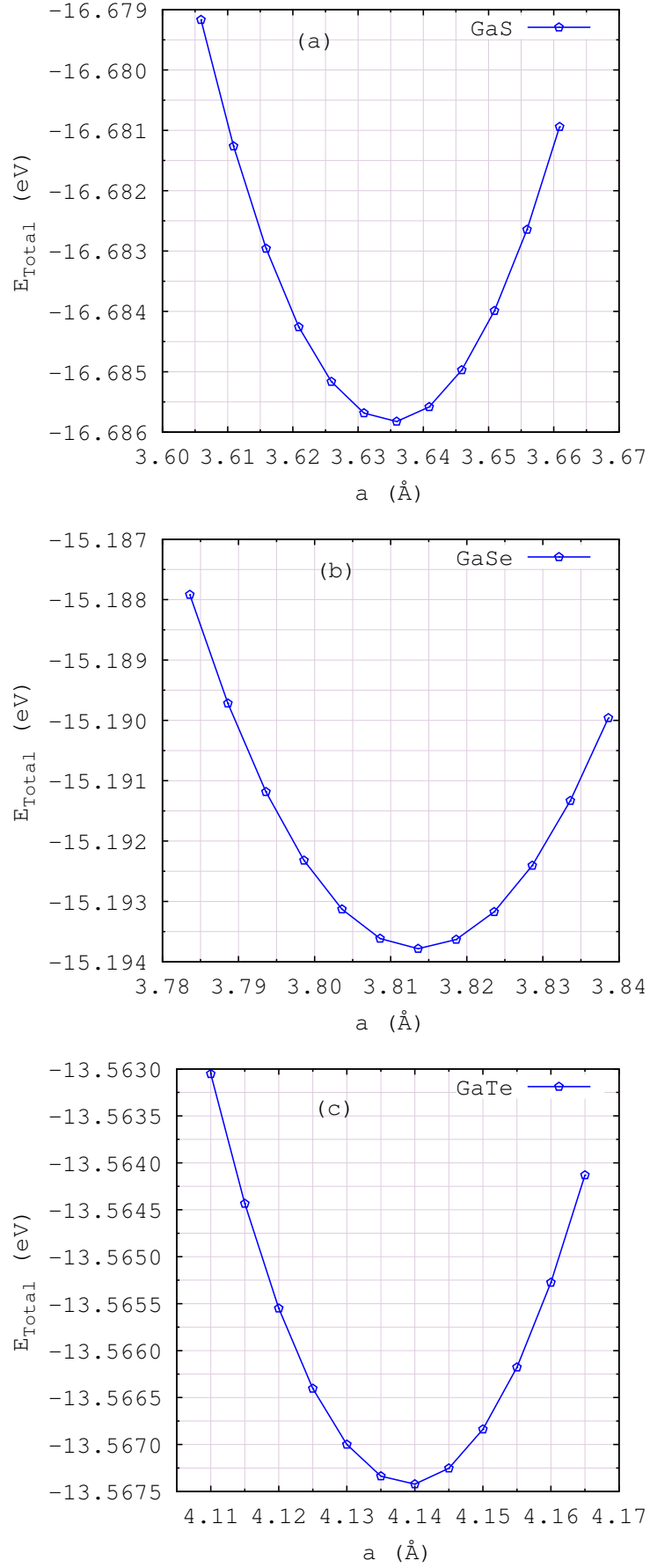


Figure S1: The total energy (eV) as a function of lattice constant a (Å). (a) GaS monolayer, (b) GaSe monolayer and (c) GaTe monolayer.

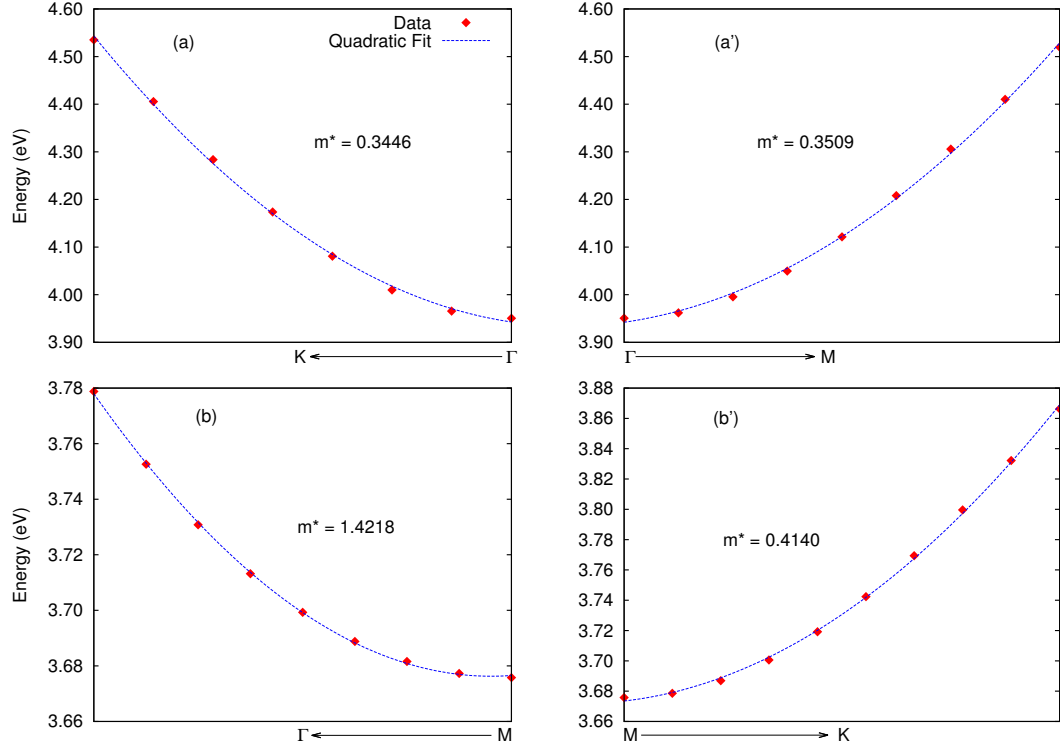


Figure S2: The fitting of quadratic equation to the E-k data of GaS monolayer. (a, a') CBM at Γ -point i.e. Γ -K and Γ -M k-path respectively. (b, b') CBM at M-point i.e. M- Γ and M-K k-path respectively.

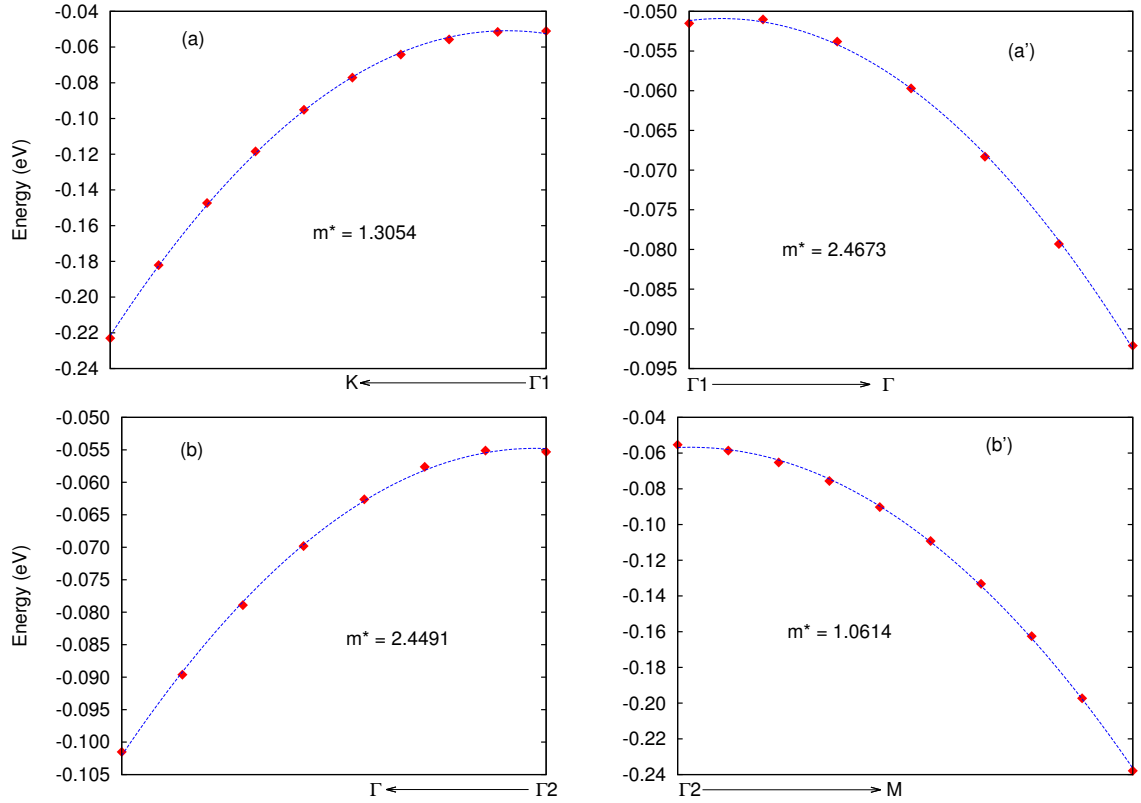


Figure S3: The fitting of quadratic equation to the E-k data of GaS monolayer. (a, a') VBM at Γ_1 -point, i.e. Γ_1 -K and Γ_1 - Γ k-path respectively. (b, b') VBM at Γ_2 -point, i.e. Γ_2 - Γ and Γ_2 -M k-path respectively.

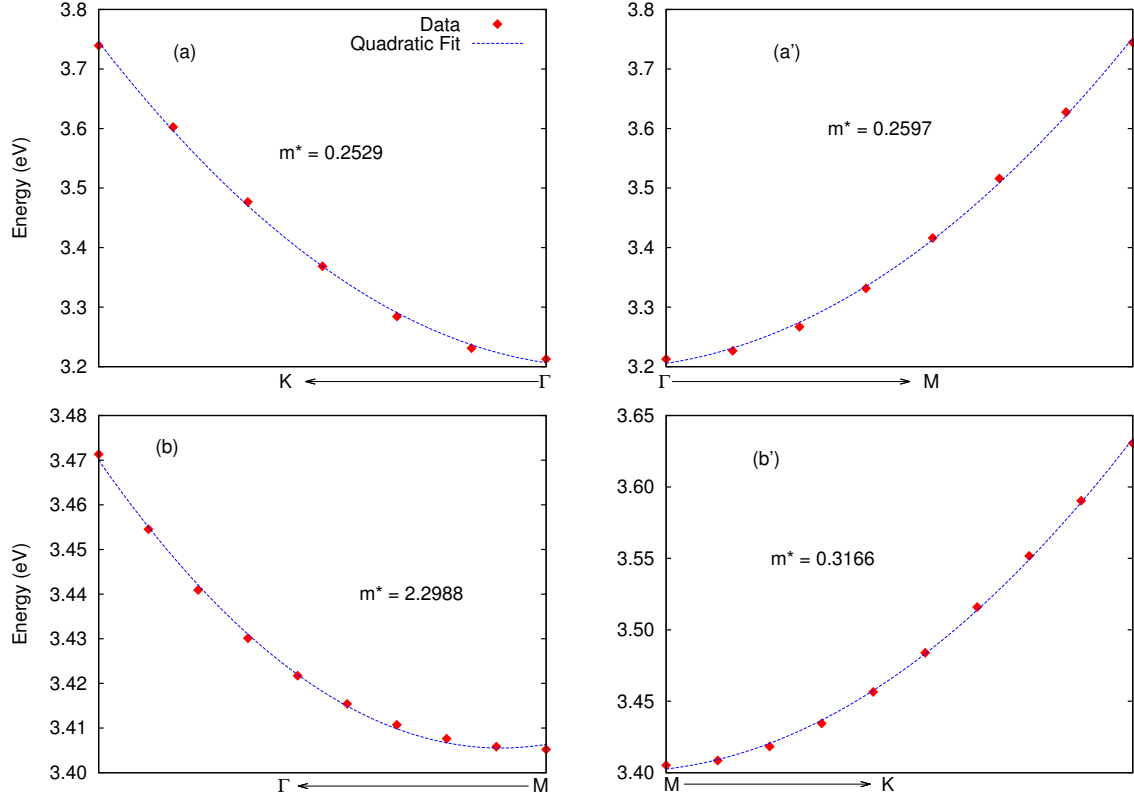


Figure S4: The fitting of quadratic equation to the E-k data of GaSe monolayer. (a, a') CBM at Γ -point i.e. Γ -K and Γ -M k-path respectively. (b, b') CBM at M-point i.e. M- Γ and M-K k-path respectively.

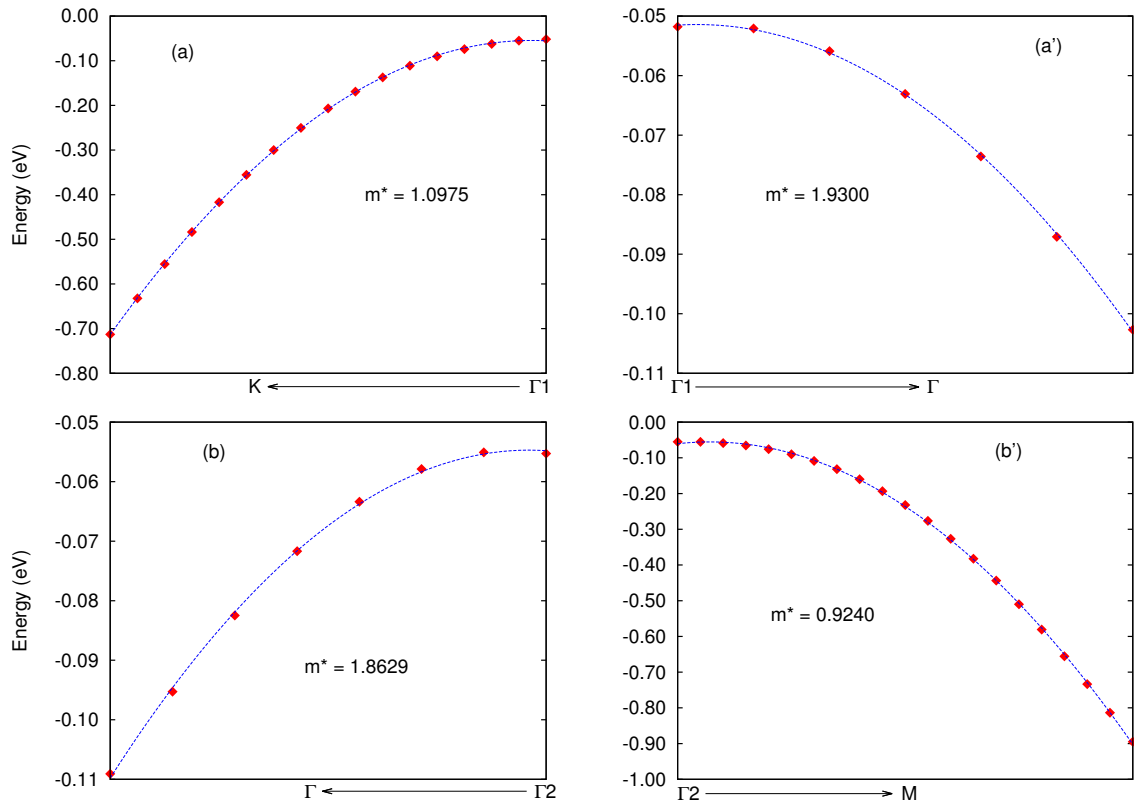


Figure S5: The fitting of quadratic equation to the E-k data of GaSe monolayer. (a, a') VBM at Γ_1 -point, i.e. Γ_1 -K and Γ_1 - Γ k-path respectively. (b, b') VBM at Γ_2 -point, i.e. Γ_2 - Γ and Γ_2 -M k-path respectively.

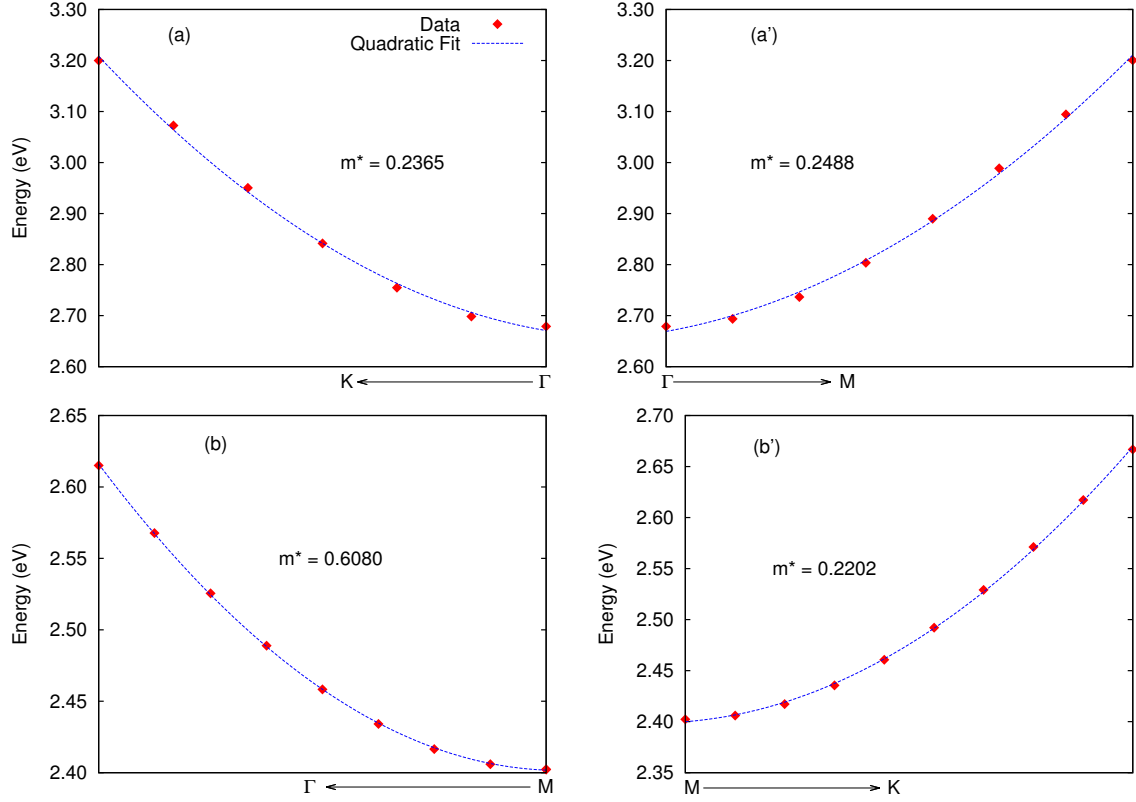


Figure S6: The fitting of quadratic equation to the E-k data of GaTe monolayer. (a, a') CBM at Γ -point i.e. Γ -K and Γ -M k-path respectively. (b, b') CBM at M-point i.e. M- Γ and M-K k-path respectively.

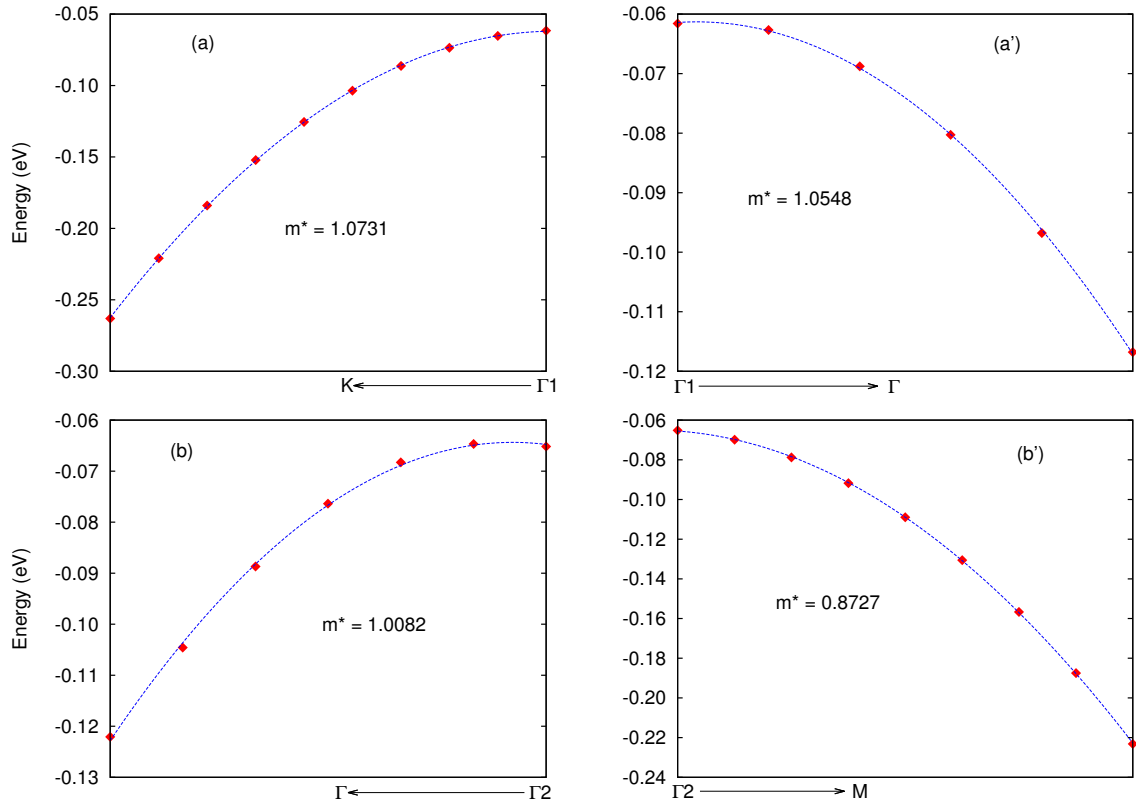


Figure S7: The fitting of quadratic equation to the E-k data of GaTe monolayer. (a, a') VBM at Γ_1 -point, i.e. Γ_1 -K and Γ_1 - Γ k-path respectively. (b, b') VBM at Γ_2 -point, i.e. Γ_2 - Γ and Γ_2 -M k-path respectively.