Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Material

Halogenation of SiGe monolayer: Robust change in electronic and thermal transports

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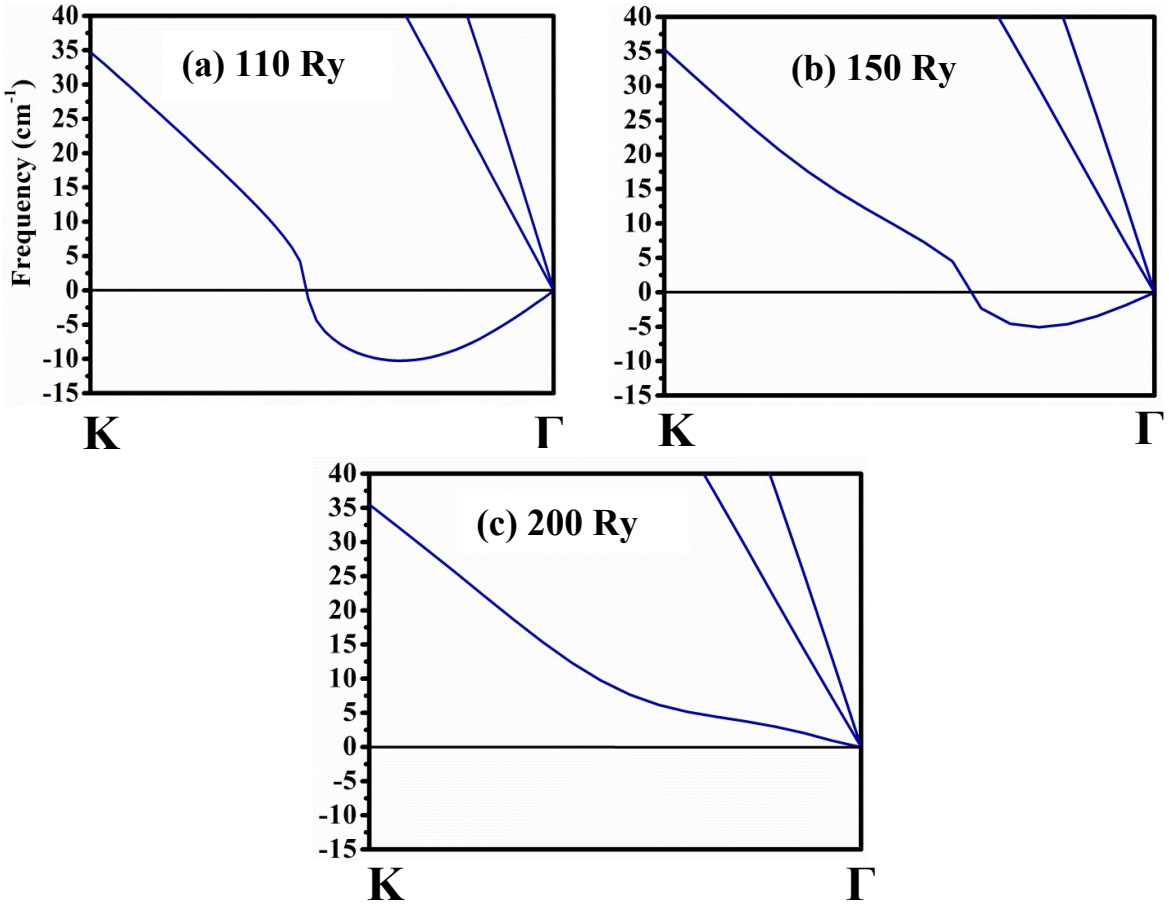


Figure S1: Phonon dispersion in K to Γ direction with different energy cut-off (a) 110Ry, (b) 150 Ry and (c) 200Ry. Increasing ecut wave function for SiGe buckled monolayer leads imaginary frequency of out-of-plane ZA mode towards the real frequency. This clearly depicts that phonon calculation is a very sensitive to the structural and calculation parameters.

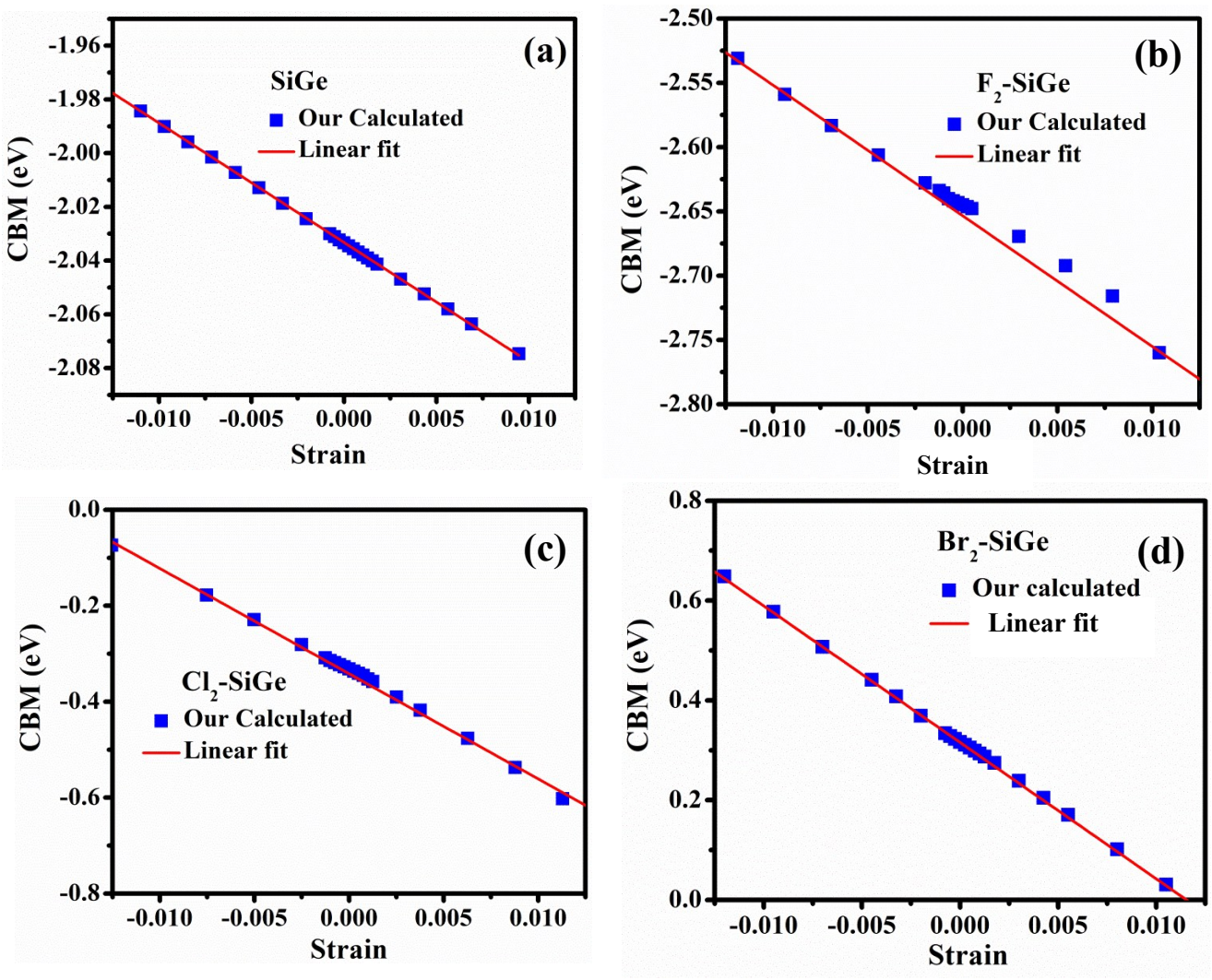
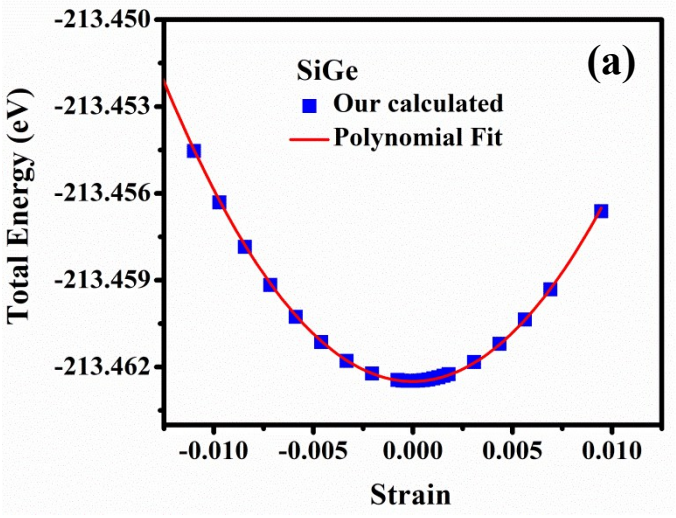
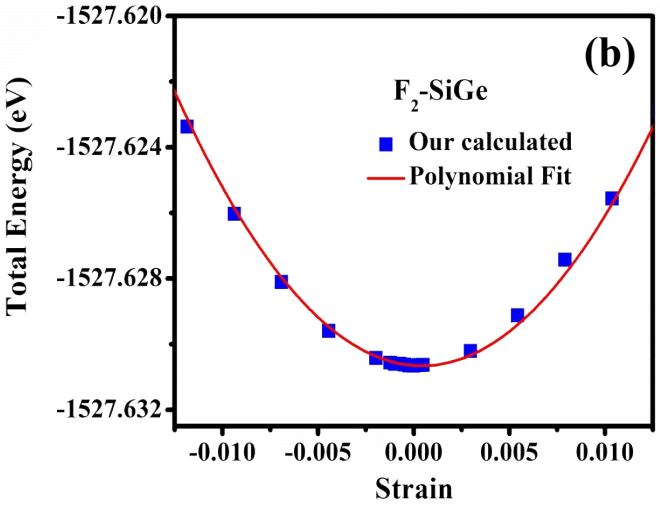
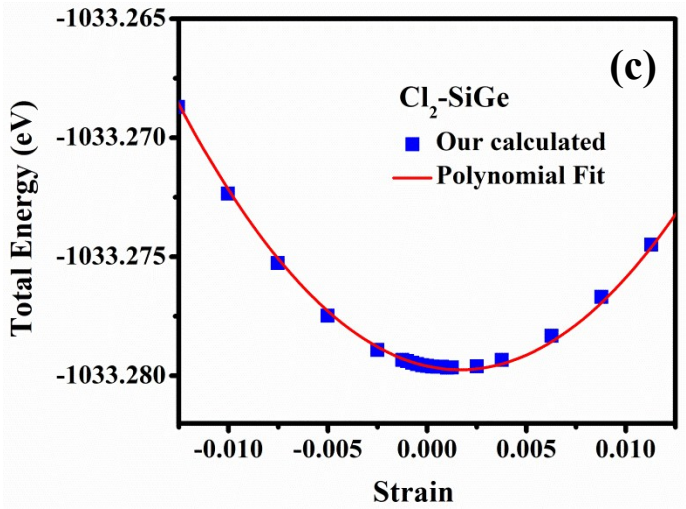


Fig S2: Strain versus conduction band minima (CBM) plots for (a) SiGe (b) F_2-SiGe (c) Cl_2-SiGe and (d) Br_2-SiGe monolayer.


(a)
SiGe
Our calculated
Polynomial Fit
Total Energy (eV)
-213.450
-213.453
-213.456
-213.459
-213.462
-0.010
-0.005
0.000
0.005
0.010
Strain


(b)
F2-SiGe
Our calculated
Polynomial Fit
Total Energy (eV)
-1527.620
-1527.624
-1527.628
-1527.632
-0.010
-0.005
0.000
0.005
0.010
Strain


(c)
Cl2-SiGe
Our calculated
Polynomial Fit
Total Energy (eV)
-1033.265
-1033.270
-1033.275
-1033.280
-0.010
-0.005
0.000
0.005
0.010
Strain

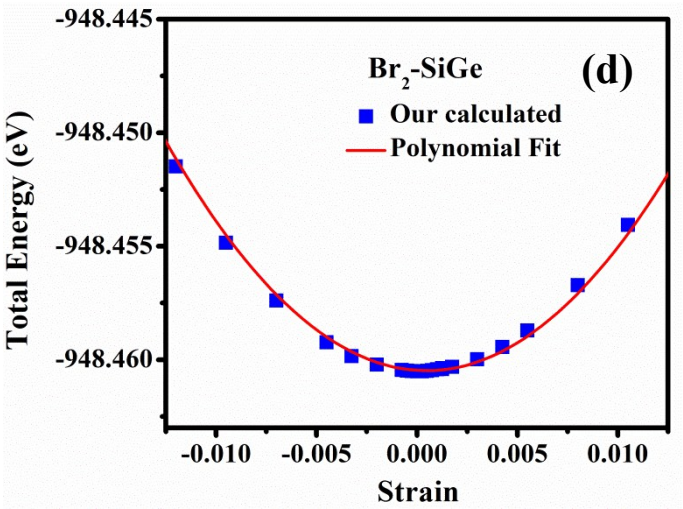

(d)
Br2-SiGe
Our calculated
Polynomial Fit
Total Energy (eV)
-948.445
-948.450
-948.455
-948.460
-0.010
-0.005
0.000
0.005
0.010
Strain

Fig S3: Strain versus total energy plots for (a) SiGe (b) F_2-SiGe (c) Cl_2-SiGe and (d) Br_2-SiGe monolayer.

Table S1: Calculated effective mass (m^*), 2D elastic constant (C^{2D}), deformation potential constant (E_1), carrier mobility (μ) and relaxation time (τ) for all considered systems at 300 K.

System	m^* (kg)	C^{2D} (N/m)	E_1 (eV)	μ ($m^2V^{-1}s^{-1}$)	τ (ps)
SiGe	2.01E-32	66.58	4.45	441.058	55.42
F_2-SiGe	2.99E-32	49.96	10.17	0.96	0.18
Cl_2-SiGe	3.58E-32	55.56	21.94	0.16	0.04
Br_2-SiGe	4.23E-32	59.95	23.34	0.11	0.03