Electronic Supplementary Information for:

Janus Zirconium Halide ZrXY (X, Y = Br, Cl & F) Monolayers with High Lattice Thermal Conductivity and Strong Visible-Light Absorption

Janpreet Singh[a,*], Gurinder Singh[b] and Surya Kant Tripathi[c]

[a]Department of Physics, Akal University, Talwandi Sabo, Punjab, 151302, India,

[b]Department of UIET, Panjab University SSG Regional Centre, Hoshiarpur, Punjab-146021, India,

[c]Department of Physics, Centre of Advanced Study in Physics, Panjab University, Chandigarh-160014, India

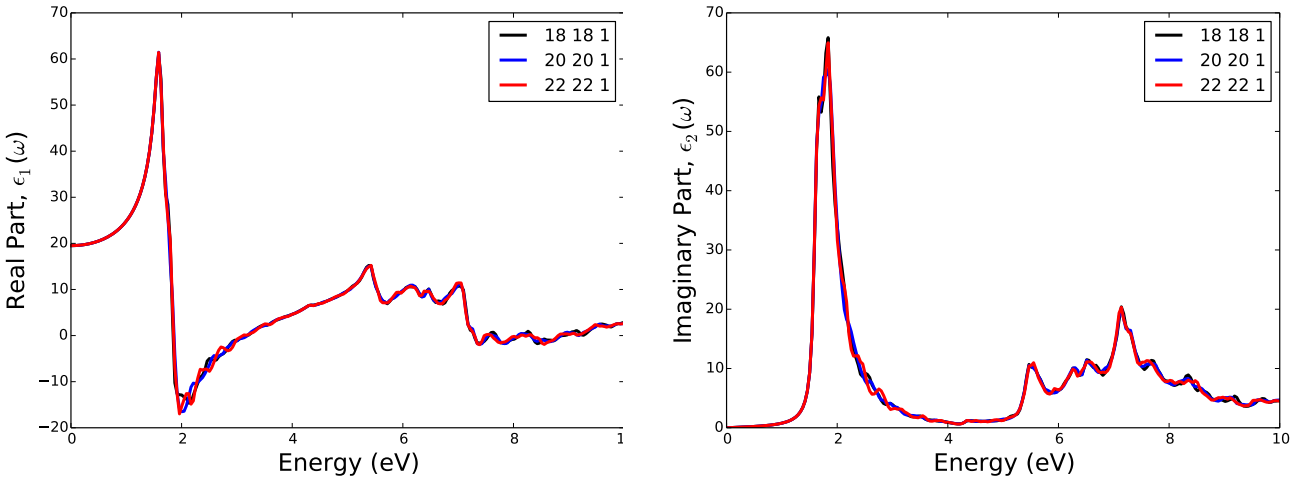
*janpreetsidhu@gmail.com

Table S1: The lattice parameters (a and b), bond lengths, bond lengths, and binding energy (E_b) of Janus ZrXY monolayers in 1T phase.

Material	a=b (Å)	Zr-Br (Å)	Zr-Cl (Å)	Zr-F (Å)	E_b (eV)
ZrBrCl	3.419	2.773	2.648	-	-4.914
ZrBrF	3.287	2.743	-	2.336	-5.430
ZrClF	3.184	-	2.608	2.315	-5.722

Table S2: The fractional ionic character (FIC) values for bonds in Janus ZrBrCl, ZrBrF, and ZrClF monolayers.

Material	Zr→Br	Zr→Cl	Zr→F
ZrBrCl	36.10	30.68	-
ZrBrF	39.96	-	27.37
ZrClF	-	37.55	29.42



(a) (b)

Figure S1: Convergence of (a) real and (b) imaginary part of dielectric constant for grid size 18×18×1, 20×20×1, and 22×22×1.

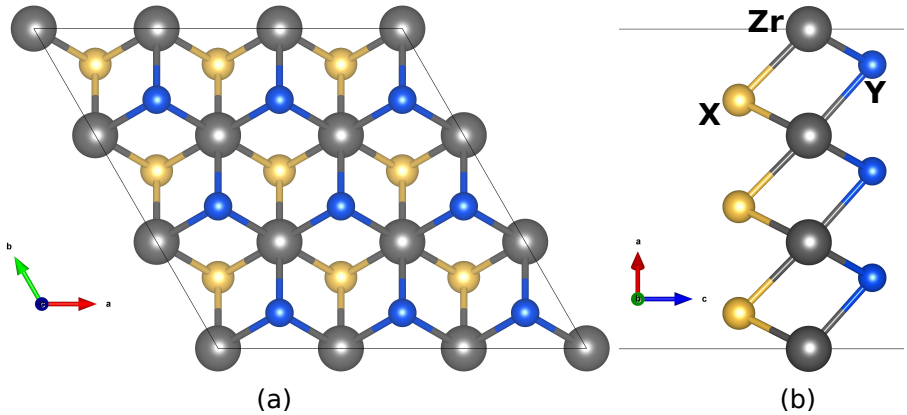


Figure S2: Top view (a) and side view (b) of the Janus ZrXY monolayer in 1T phase. Here X, Y=Br, Cl, F

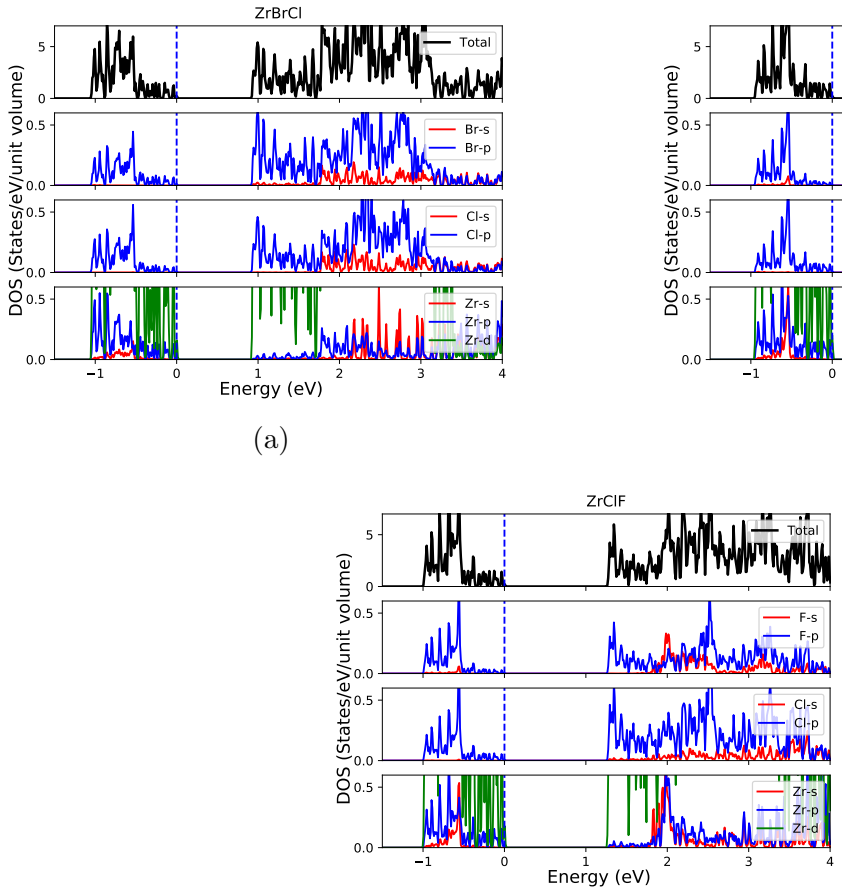


Figure S3: The atom-projected density of states for (a) ZrBrCl, (b) ZrBrF, and (c) ZrClF.

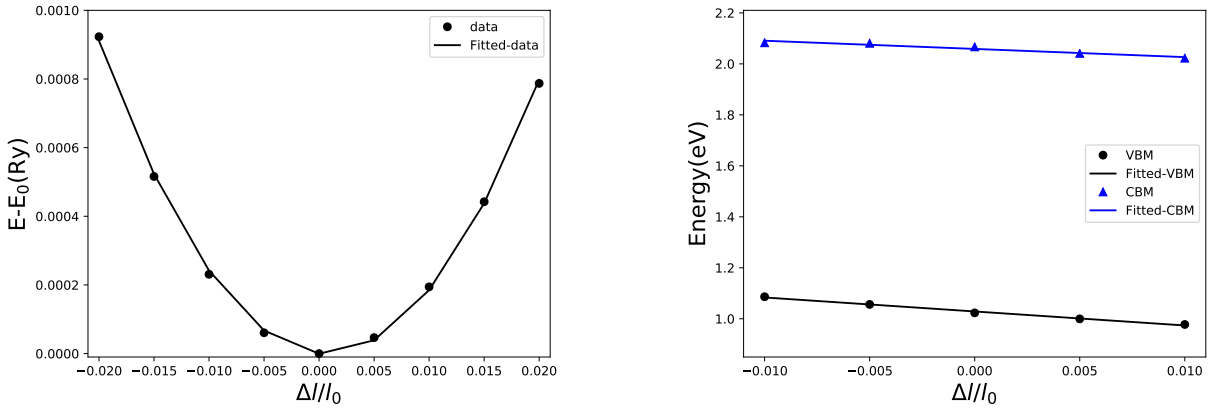
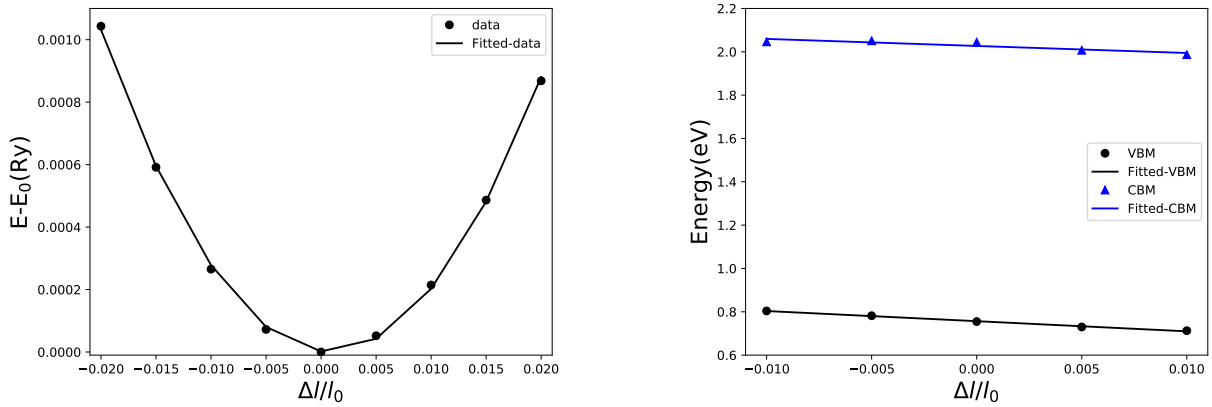
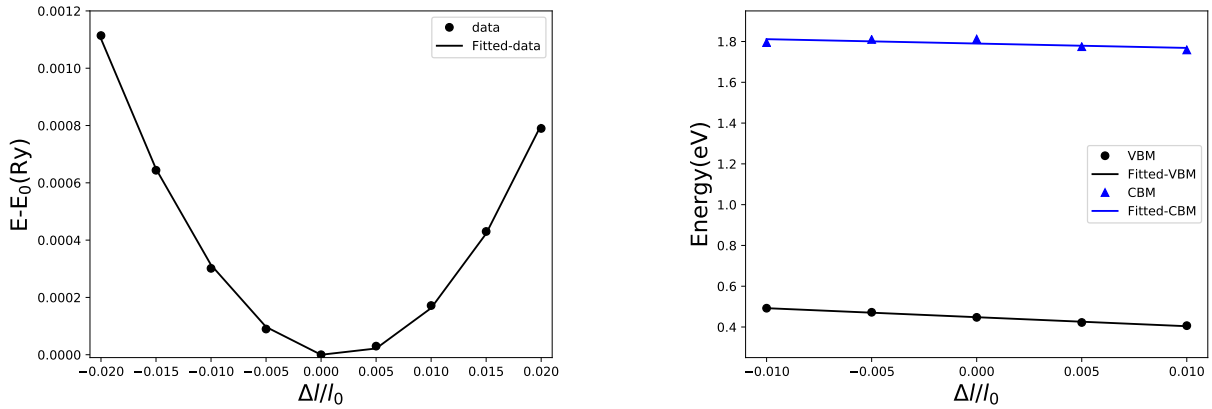


Figure S4: (a) Graph and parabolic fit between energy and strain, (b) Graph and straight fit graph between band edges (E_{CBM}, and E_{VBM}) and strain for ZrBrCl monolayer.



(a) (b)

Figure S5: (a) Graph and parabolic fit between energy and strain, (b) Graph and straight fit graph between band edges (E_{CBM}, and E_{VBM}) and strain for ZrBrF monolayer.



(a) (b)

Figure S6: (a) Graph and parabolic fit between energy and strain, (b) Graph and straight fit graph between band edges (E_{CBM}, and E_{VBM}) and strain for ZrClF monolayer.

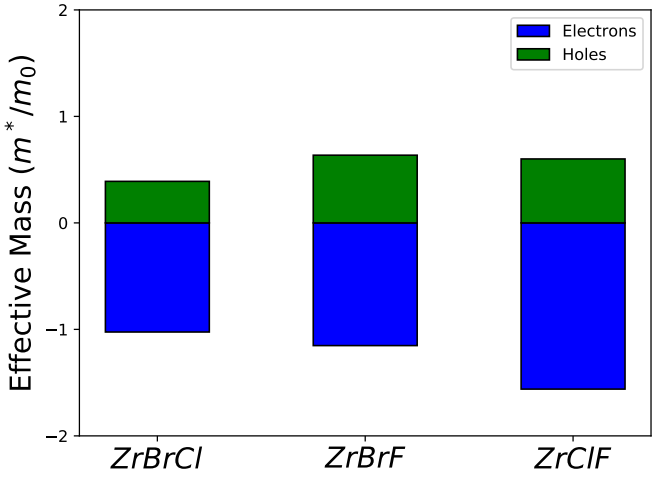


Figure S7: Effective mass of electrons and holes determined using slope method.

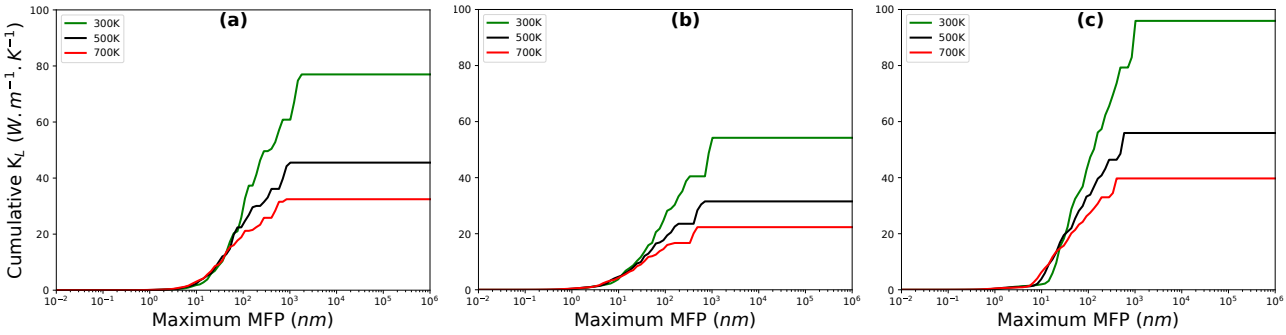


Figure S8: The cumulative lattice thermal conductivity with respect to the mean free path of (a) ZrBrCl, (b) ZrBrF, and (c) ZrClF monolayer at 300 K, 500 K and 700 K.