Supplementary Information:
Flexoelectricity in atomic monolayers from first principles

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Table 1 Equilibrium geometry for the atomic monolayers with honeycomb lattice structure. The atom positions are $\boldsymbol{R} = f_1\boldsymbol{a_1} + f_2\boldsymbol{a_2} + \Delta\hat{\boldsymbol{e}}_3$, where $\boldsymbol{a_1} = \frac{a}{2}\hat{\boldsymbol{e}}_1 + \frac{\sqrt{3}a}{2}\hat{\boldsymbol{e}}_2$ and $\boldsymbol{a_2} = \frac{-a}{2}\hat{\boldsymbol{e}}_1 + \frac{\sqrt{3}a}{2}\hat{\boldsymbol{e}}_2$, with $\hat{\boldsymbol{e}}_1$, $\hat{\boldsymbol{e}}_2$, and $\hat{\boldsymbol{e}}_3$ being the unit vectors along the x_1, x_2, and x_3 directions, respectively.

Group	Material	Lattice parameter a (Bohr)	Atom positions $(f_1, f_2, \Delta$(Bohr)$)$
Group III monochalcogenides (h1)	GaS	6.89	Ga: (0.00, 0.00, -2.34), (0.00, 0.00, 2.34) S: (0.33, 0.67,-4.37), (0.33, 0.67, 4.37)
	GaSe	7.18	Ga: (0.00, 0.00,-2.34), (0.00, 0.00,2.34) Se: (0.33, 0.67,-4.58), (0.33, 0.67, 4.58)
	GaTe	7.74	Ga: (0.00, 0.00,- 2.32). (0.00, 0.00, 2.32) Te: (0.33, 0.67, -4.76), (0.33, 0.67,4.76)
	InS	7.41	Ga: (0.00, 0.00, -2.19). (0.00, 0.00,2.19) Te: (0.33, 0.67,-4.90), (0.33, 0.67,4.90)
	InSe	7.70	In: (0.00, 0.00,-2.66), (0.00, 0.00, 2.66) Se: (0.33, 0.67,-5.07), (0.33, 0.67,5.07)
	InTe	8.26	In: (0.00, 0.00,-2.66), (0.00, 0.00,2.66) Se: (0.33, 0.67,-5.27), (0.33, 0.67,5.27)
Transition metal dichalcogenides (h2)	TiS_2	6.45	Ti: (0.00, 0.00, 0.00) S: (0.33, 0.66, 2.68), (0.66, 0.33, -2.68)
	$TiSe_2$	6.68	Ti: (0.00, 0.00, 0.00) Se: (0.33, 0.67, 2.93), (0.67, 0.33, -2.93)
	$TiTe_2$	7.08	Ti: (0.00, 0.00, 0.00) Se: (0.33, 0.67, 3.31), (0.67, 0.33, -3.31)
	ZrS_2	6.96	Zr: (0.00, 0.00, 0.00) S: (0.33, 0.67, 2.74), (0.67, 0.33, -2.74)
	$ZrSe_2$	7.17	Zr: (0.00, 0.00, 0.00) Se: (0.33, 0.67, 3.00), (0.67, 0.33, -3.00)
	$ZrTe_2$	7.50	Zr: (0.00, 0.00, 0.00) Se: (0.33, 0.67, 3.40), (0.67, 0.33, -3.40)
	MoS_2	6.02	Mo: (0.00, 0.00, 0.00) S: (0.33, 0.33, 2.96), (0.33, 0.33, -2.96)
	$MoSe_2$	6.31	Mo: (0.00, 0.00, 0.00) Se: (0.33, 0.33, 3.14), (0.33, 0.33, -3.14)

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Table 1. – *Continued.*

Group	Material	Lattice parameter a (Bohr)	Atom positions $(f_1, f_2, \Delta$(Bohr))
	$MoTe_2$	6.68	Mo: (0.00, 0.00, 0.00) Se: (0.33, 0.33, 3.45), (0.33, 0.33, −3.45)
	WS_2	6.02	W: (0.00, 0.00, 0.00) S: (0.33, 0.33, 2.97), (0.33, 0.33, −2.97)
	WSe_2	6.28	W: (0.00, 0.00, 0.00) Se: (0.33, 0.33, 3.17), (0.33, 0.33, −3.17)
	WTe_2	6.67	W: (0.00, 0.00, 0.00) Se: (0.33, 0.33, 3.46), (0.33, 0.33, −3.46)
	NbS_2	6.33	Nb: (0.00, 0.00, 0.00) S: (0.33, 0.33, 2.96), (0.33, 0.33, −2.96)
	$NbSe_2$	6.57	Nb: (0.00, 0.00, 0.00) Se: (0.33, 0.33, 3.17), (0.33, 0.33, −3.17)
	$NbTe_2$	6.99	Nb: (0.00, 0.00, 0.00) Te: (0.33, 0.33, 3.48), (0.33, 0.33, −3.48)
	HfS_2	6.90	Hf: (0.00, 0.00, 0.00) S: (0.33, 0.67, 2.74), (0.67, 0.33, −2.74)
Group IV, III-V monolayers (h3)	C	4.65	C: (0.00, 0.00, 0.00), (0.33, 0.33, 0.00)
	Si	7.31	Si: (0.00, 0.00, 0.00), (0.33, 0.33, 0.86)
	Ge	7.65	Ge: (0.00, 0.00, -0.64), (0.33, 0.33, 0.64)
	Sn	8.84	Sn: (0.00, 0.00, -0.81), (0.33, 0.33, 0.81)
	BN	4.74	B: (0.00, 0.00, 0.00); N: (0.33, 0.33, 0.00)
Group V monolayers (h3)	P	6.20	P: (0.00, 0.00, 0.00), (0.33, 0.33, 1.17)
	As	6.82	As: (0.00, 0.00, 0.00), (0.33, 0.33, 1.17)
	Sb	7.78	Sb: (0.00, 0.00, 0.00), (0.33, 0.33, 1.55)
	Bi	8.22	Bi: (0.00, 0.00, 0.00), (0.33, 0.33, 1.63)
Group IV dichalcogenides (h4)	GeS_2	6.50	Ge: (0.00, 0.00, 0.00) S: (0.33, 0.67, 2.64), (0.67, 0.33, −2.64)
	$GeSe_2$	6.85	Ge: (0.00, 0.00, 0.00) Se: (0.33, 0.67, 2.87), (0.67, 0.33, −2.87)
	SnS_2	7.00	Sn: (0.00, 0.00, 0.00) S: (0.33, 0.67, 2.80), (0.67, 0.33, −2.80)
	$SnSe_2$	7.32	Sn: (0.00, 0.00, 0.00) Se: (0.33, 0.67, 3.01), (0.67, 0.33, −3.01)

Table 2 Equilibrium geometry for the atomic monolayers with rectangular lattice structure. The atom positions are $\boldsymbol{R} = f_1\boldsymbol{a_1} + f_2\boldsymbol{a_2} + \Delta\hat{\boldsymbol{e}}_3$, where $\boldsymbol{a_1} = a_1\hat{\boldsymbol{e}}_1$ and $\boldsymbol{a_2} = a_2\hat{\boldsymbol{e}}_2$, with $\hat{\boldsymbol{e}}_1$, $\hat{\boldsymbol{e}}_2$ and $\hat{\boldsymbol{e}}_3$ being the unit vectors along the x_1, x_2 and x_3 directions, respectively.

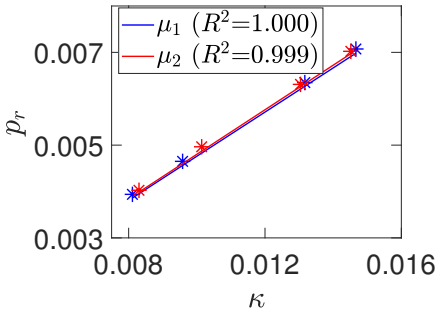
Group	Material	Lattice parameters (Bohr)	Atom positions $(f_1,\ f_2, \Delta$(Bohr))
Group V monolayers (t1)	P	$a_1 = 8.75$ $a_2 = 6.24$	P: (0.00, 0.00, 0.00), (0.18, 0.00, 3.98) (0.51, 0.50, 3.98), (0.68, 0.50, 0.00)
	As	$a_1 = 9.01$ $a_2 = 6.95$	As: (0.00, 0.00, 0.00), (0.14, 0.00, 4.54) (0.49, 0.50, 4.54), (0.66, 0.50, 0.00)
	Sb	$a_1 = 8.54$ $a_2 = 8.34$	Sb: (0.78, 0.75, 2.13), (0.36, 0.25, 3.15) (0.64, 0.75, -2.13), (0.21, 0.25, -3.15)
	Bi	$a_1 = 9.52$ $a_2 = 8.34$	Bi: (0.79,0.75,2.21), (0.37, 0.35, 3.36) (0.63, 0.75, -3.36), (0.21, 0.25, 2.21)
Group IV monochalogenides (t1)	GeS	$a_1 = 8.48$ $a_2 = 6.91$	Ge: (0.03 0.00, 2.03), (0.53, 0.50, -2.03) S: (0.16, 0.00, -2.41), (0.67,0.50,2.41)
	GeSe	$a_1 = 8.58$ $a_2 = 7.34$	Ge: (0.13, 0.00, -2.34), (0.61, 0.50, 2.34) Se: (0.50, 0.50, -2.37), (0.00, 0.00, 2.37)
	SnS	$a_1 = 8.12$ $a_2 = 7.73$	Sn: (0.39,0.00,-2.68), (0.89, 0.50, 2.68) S: (0.97, 0.50, -2.19), (0.47, 0.00, 2.19)
	SnSe	$a_1 = 8.58$ $a_2 = 8.00$	Sn: (0.41, 0.00, -2.62), (0.91, 0.50, 2.62) Se: (0.98, 0.50, -2.50), (0.48, 0.00, 2.50)
Transition metal trichalcogenides (t2)	ZrS_3	$a_1 = 9.81$ $a_2 = 6.90$	Zr: (0.63,0.25,2.61), (0.13, 0.75, -2.61) S: (0.13, 0.25, 0.92), (0.63, 0.75,- 0.92) (0.33, 0.25, -5.58), (0.43, 0.75, 5.58) (-0.06, 0.25, -5.58), (0.83, 0.75, 5.58)
	$ZrSe_3$	$a_1 = 10.34$ $a_2 = 7.16$	Zr: (0.63, 0.25, 2.81), (0.13, 0.75, -2.81) Se: (0.13, 0.25, 0.96), (0.63, 0.75, -0.96) (0.33, 0.25, -5.88), (0.43, 0.75, 5.88) (-0.09, 0.25, -5.88), (0.83, 0.75, 5.88)
	TiS_3	$a_1 = 9.50$ $a_2 = 6.48$	Ti: (0.63,0.25,2.53), (0.13, 0.75, -2.53) S: (0.13, 0.25, 0.83), (0.63, 0.75, -0.83) (0.33, 0.25, -5.37), (0.43, 0.75, 5.37) (-0.07, 0.25, -5.37), (0.83, 0.75, 5.37)
	HfS_3	$a_1 = 9.74$ $a_2 = 6.84$	Hf: (0.63, 0.25, 2.61), (0.13, 0.75, -2.61) S: (0.13, 0.25, 0.90), (0.63, 0.75, -0.90) (0.34, 0.25, -5.56), (0.43, 0.75, 5.56) (-0.07, 0.25, -5.56), (0.84, 0.75, 5.56)
	$HfSe_3$	$a_1 = 10.30$ $a_2 = 7.09$	Hf: (0.63, 0.25, 2.79), (0.13, 0.75, -2.79) Se: (0.13, 0.25, 0.95), (0.63, 0.75, -0.95) (0.35, 0.25, -5.85), (0.41, 0.75, 5.85) (-0.09, 0.25, -5.85), (0.85, 0.75, 5.85)
	$ZrTe_3$	$a_1 = 11.22$ $a_2 = 7.51$	Zr: (0.63,0.25,3.24), (0.13, 0.75, -3.24) Te: (0.13, 0.25, 1.00), (0.63, 0.75, -1.00) (0.33, 0.25, -6.41), (0.43, 0.75, 6.41) (-0.11, 0.25, -6.41), (0.83, 0.75, 6.41)

Table 2. – *Continued.*

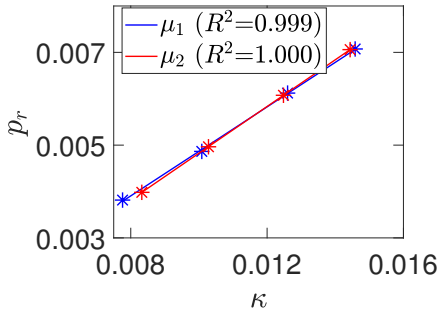
Group	Material	Lattice parameters (Bohr)	Atom positions (f_1, f_2, Δ(Bohr))
Group V chalcogenides (t3)	As_2S_3	$a_1 = 7.92$ $a_2 = 21.87$	As: (-0.18, -0.33, 1.22), (0.31, -0.11, -1.22) (0.31, 0.17, -1.22), (-0.19, 0.39, 1.22) S: (0.17, 0.25, 2.56), (-0.33, -0.25, -2.56) (-0.33, 0.31, -2.56), (0.17, -0.19, 2.56) (-0.37, 0.03, 0.65), (0.13, -0.47, -0.65)
	As_2Se_3	$a_1 = 7.73$ $a_2 = 22.96$	As: (0.60, 0.01, 1.13), (0.10, 0.24, -1.12) (0.10, 0.51, -1.13), (0.60, 0.74, 1.12) Se: (0.48, 0.10, -2.86), (0.98, 0.60, 2.96) (0.98, 0.15, 2.86), (0.48, 0.65, -2.86) (0.46, 0.37, 1.05), (0.96, 0.87, -1.05)
	As_2Te_3	$a_1 = 8.17$ $a_2 = 24.86$	As: (0.59, 0.10, 1.27), (0.10, 0.24, -1.27) (0.10, 0.51, -1.26), (0.59, 0.74, 1.27) Te: (0.48, 0.09, -3.09), (0.98, 0.59, 3.09) (0.98, 0.15, 3.09), (0.48, 0.65, -3.09) (0.47, 0.37, 1.11), (0.97, 0.87, -1.11)
	P_2S_3	$a_1 = 8.89$ $a_2 = 20.04$	P: (-0.15, -0.32, 1.18), (0.35, -0.11, -1.17) (0.35, 0.18, -1.18), (-0.15, 0.39, 1.17) S: (0.17, 0.25, 2.26), (-0.34, -0.25, -2.26) (-0.33, 0.31, -2.28), (0.16, -0.19, 2.28) (-0.41, 0.03, 0.64), (0.09, -0.47, -0.64)
	P_2Se_3	$a_1 = 9.01$ $a_2 = 21.65$	P: (-0.15, -0.32, 1.22), (0.34, -0.11, -1.22) (0.35, 0.18, -1.23), (-0.15, 0.39, 1.22) Se: (0.17, 0.25, 2.50), (-0.34, -0.25, -2.50) (-0.33, 0.32, -2.51), (0.16, -0.18, 2.50) (-0.39, 0.03, 0.71), (0.11, -0.46, -0.69)

Table 3 Unrelaxed transversal flexoelectric coefficient along principal directions for the fifty-four select atomic monolayers from first principles DFT calculations.

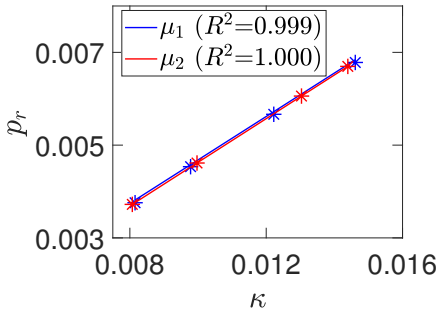
Group	Material	Flexoelectric coefficient (e)		Group	Material	Flexoelectric coefficient (e)	
		μ_1	μ_2			μ_1	μ_2
Group III monochalcogenides (h1)	GaS	0.55	0.52	Group V monolayers (h3)	P	0.25	0.25
	GaSe	0.54	0.53		As	0.26	0.27
	InS	0.56	0.58		Bi	0.33	0.33
	InSe	0.52	0.50		Sb	0.34	0.34
	InTe	0.64	0.65	Group IV dichalcogenides (h4)	$GeSe_2$	0.44	0.43
	GaTe	0.63	0.62		GeS_2	0.45	0.43
Transition metal dichalcogenides (h2)	ZrS_2	0.45	0.45		$SnSe_2$	0.40	0.41
	TiS_2	0.45	0.45		SnS_2	0.43	0.42
	$ZrSe_2$	0.46	0.47	Group V monolayers (t1)	P	0.31	0.33
	$TiSe_2$	0.41	0.40		As	0.31	0.31
	NbS_2	0.51	0.52		Bi	0.51	0.51
	$NbSe_2$	0.51	0.54		Sb	0.54	0.54
	HfS_2	0.57	0.56	Group IV monochalcogenides (t1)	GeSe	0.34	0.33
	$ZrTe_2$	0.55	0.54		GeS	0.39	0.35
	$TiTe_2$	0.58	0.56		SnSe	0.38	0.36
	$MoSe_2$	0.57	0.57		SnS	0.40	0.39
	MoS_2	0.57	0.58	Transition metal trichalcogenides (t2)	ZrS_3	0.72	0.71
	WS_2	0.59	0.59		TiS_3	0.65	0.61
	WSe_2	0.59	0.58		$ZrSe_3$	0.72	0.69
	$NbTe_2$	0.64	0.67		HfS_3	0.87	0.86
	$MoTe_2$	0.71	0.72		$HfSe_3$	0.85	0.77
	WTe_2	0.73	0.74		$ZrTe_3$	0.98	1.05
Group IV, III-V monolayers (h3)	Si	0.19	0.19	Group V chalcogenides (t3)	P_2S_3	0.25	0.26
	BN	0.20	0.20		P_2Se_3	0.26	0.29
	C	0.22	0.22		As_2S_3	0.28	0.31
	Sn	0.26	0.25		As_2Se_3	0.30	0.33
	Ge	0.27	0.27		As_2Te_3	0.43	0.42



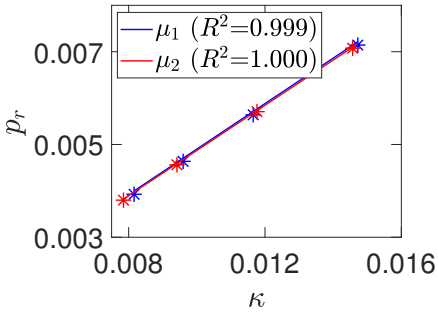
(1) GaS



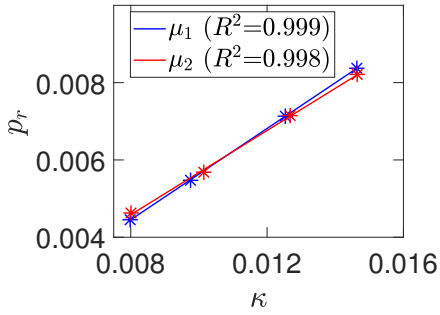
(2) GaSe



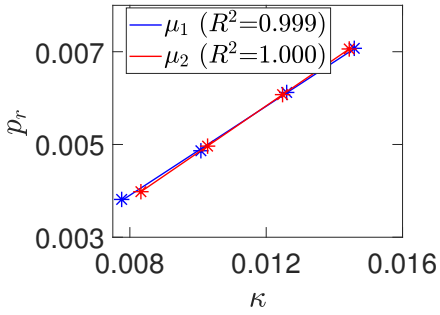
(3) InS



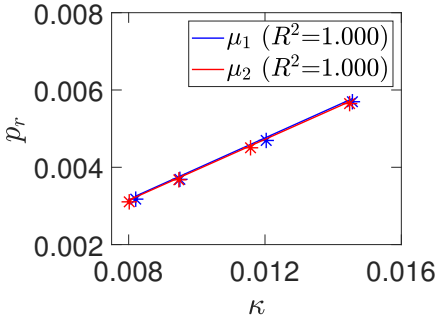
(4) InSe



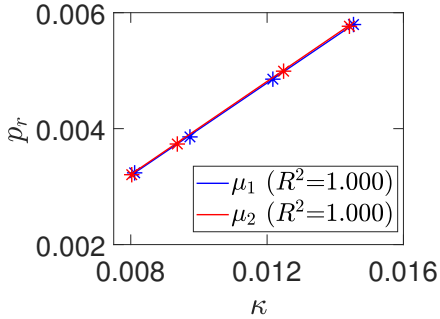
(5) InTe



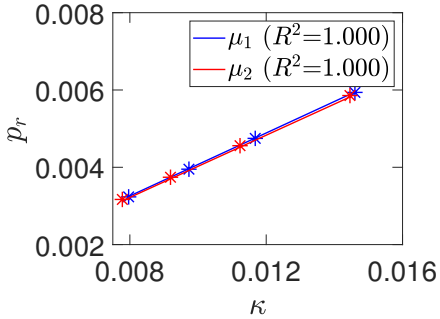
(6) GaTe



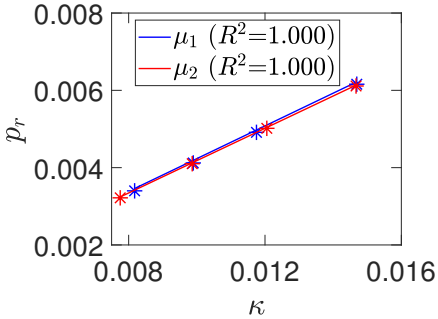
(7) ZrS_2



(8) TiS_2



(9) $ZrSe_2$



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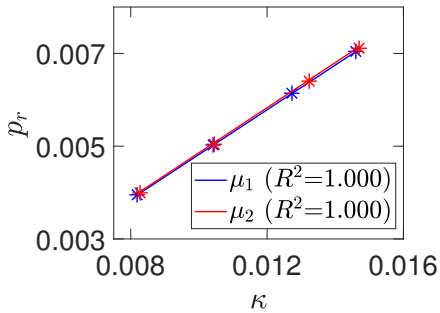
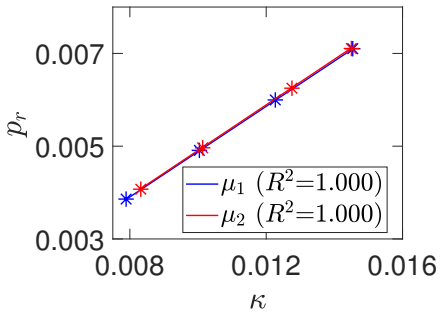
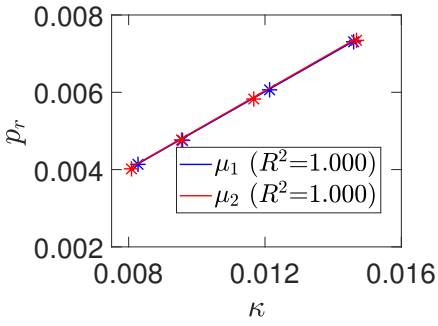


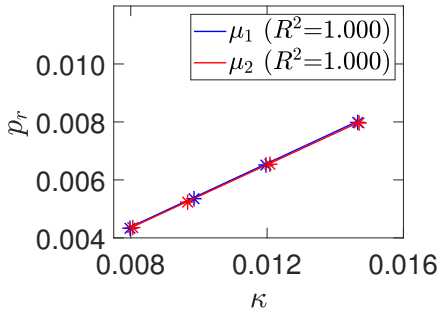
(11) NbS_2



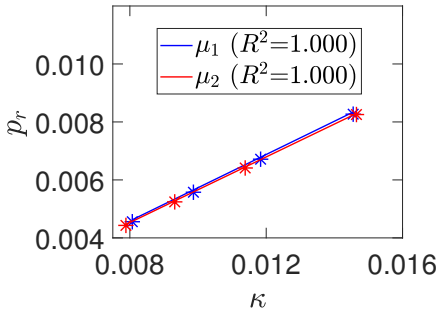
(12) $NbSe_2$



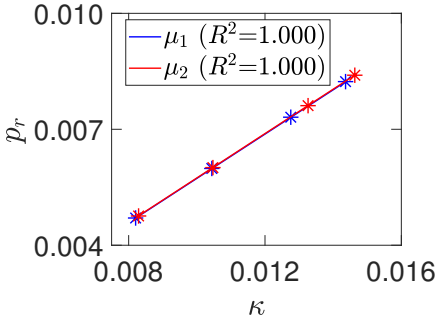
(13) HfS_2



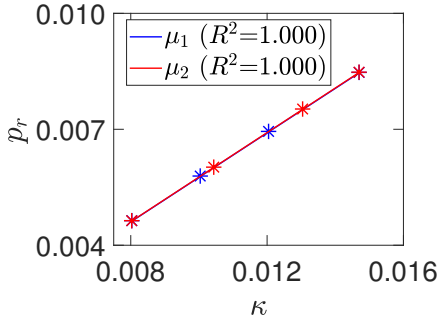
(14) $ZrTe_2$



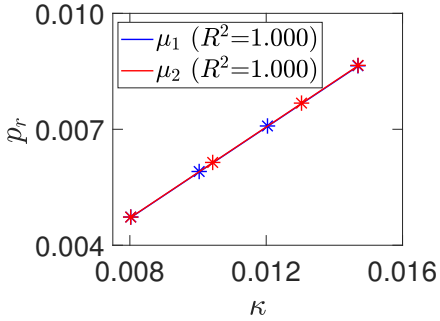
(15) $TiTe_2$



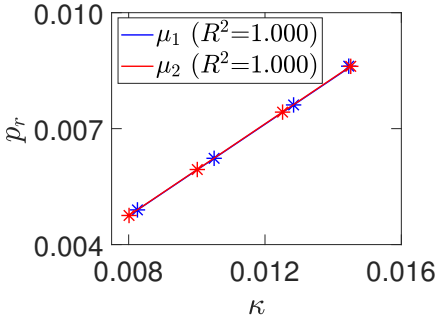
(16) $MoSe_2$



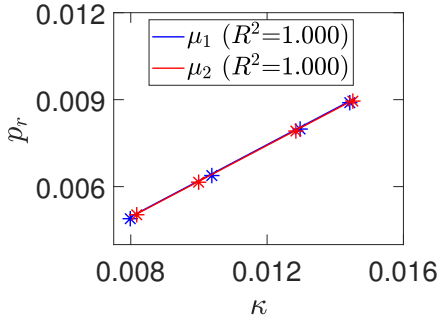
(17) MoS_2



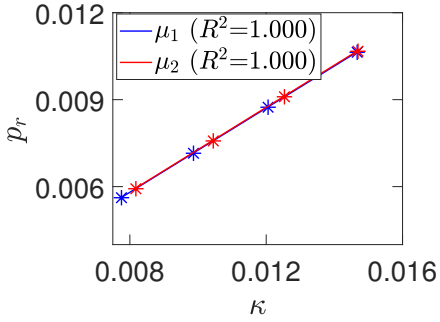
(18) WS_2



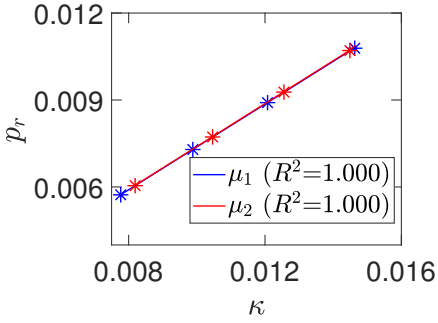
(19) WSe_2



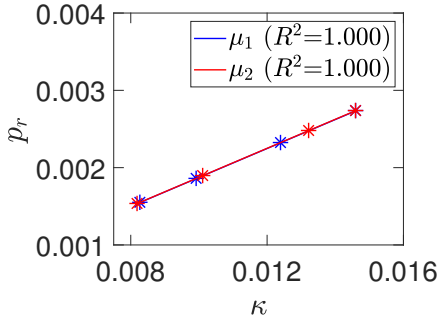
(20) $NbTe_2$



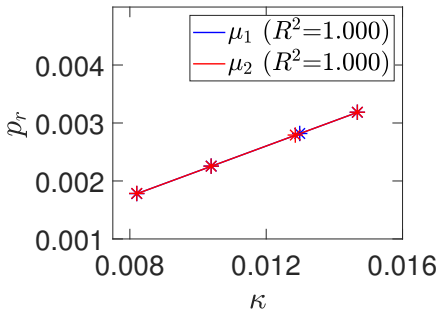
(21) $MoTe_2$



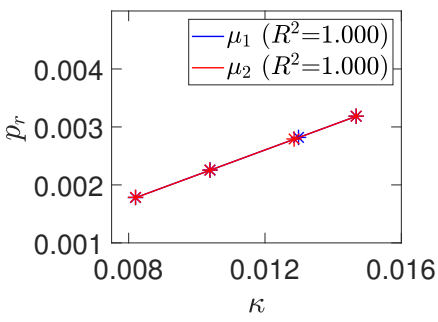
(22) WTe_2



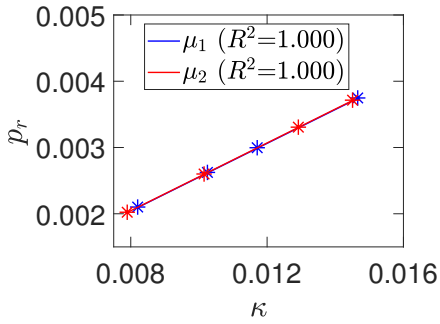
(23) Si



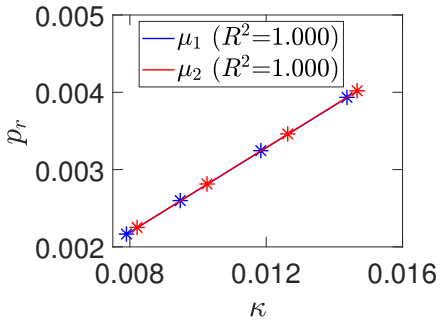
(24) BN



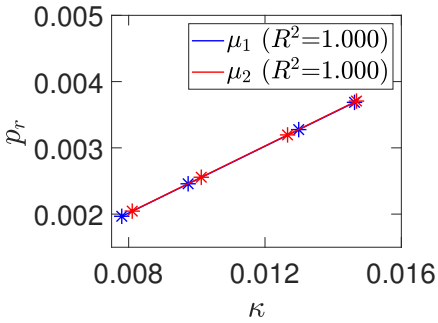
(25) C



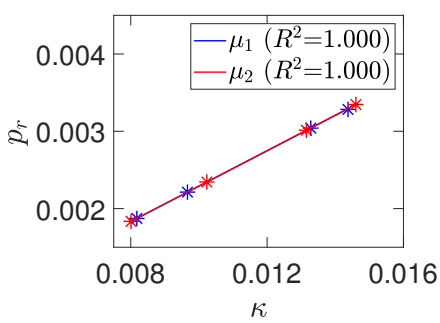
(26) Sn



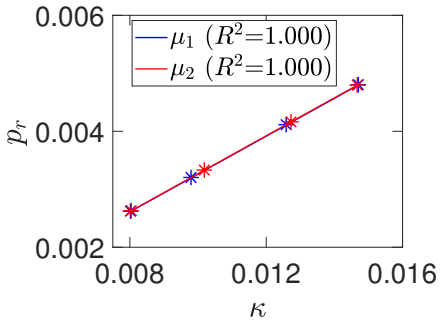
(27) Ge



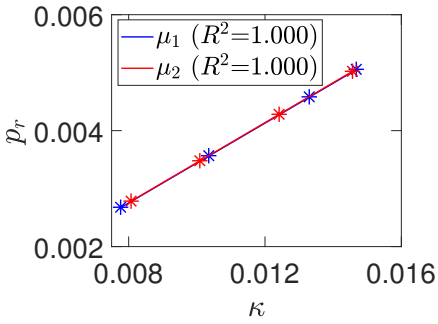
(28) P (h3)



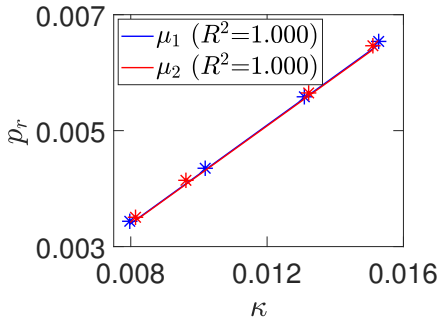
(29) As (h3)



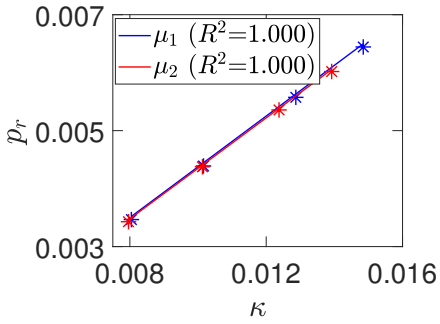
(30) Bi (h3)



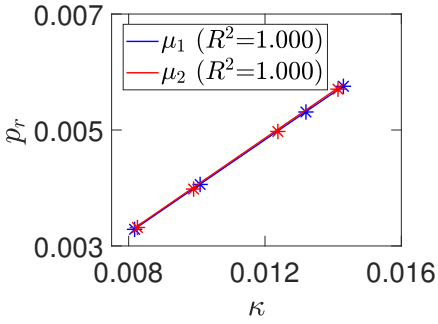
(31) Sb (h3)



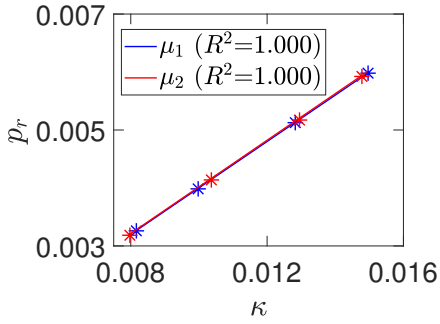
(32) $GeSe_2$



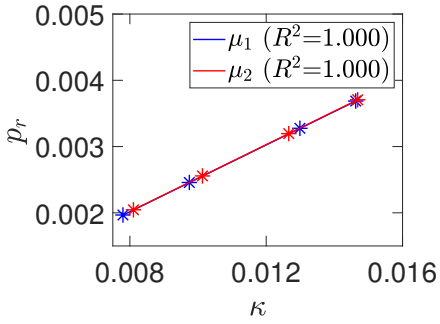
(33) GeS_2



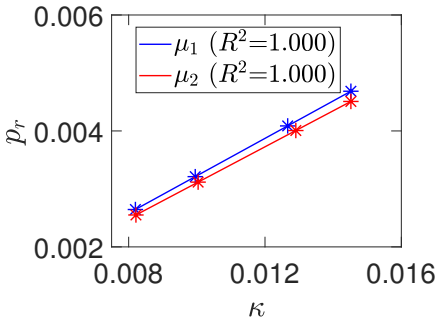
(34) $SnSe_2$



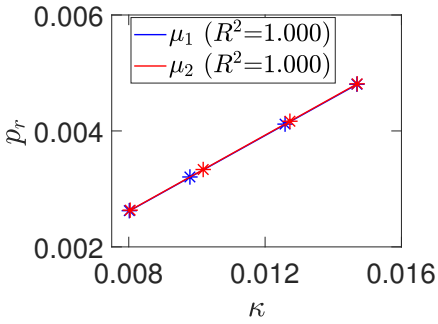
(35) SnS_2



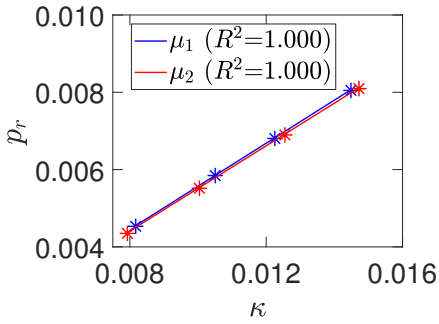
(36) P (t1)



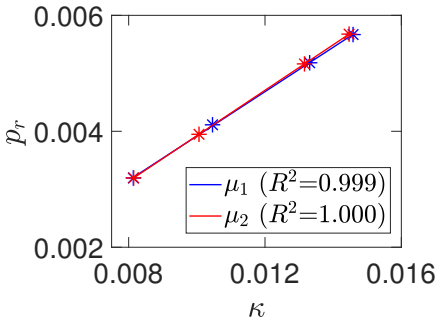
(37) As (t1)



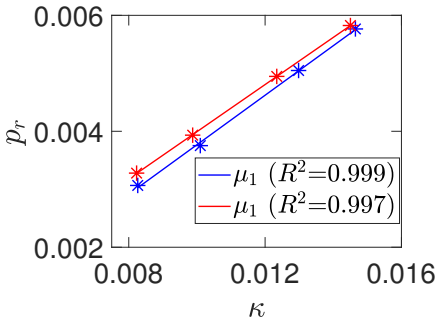
(38) Bi (t1)



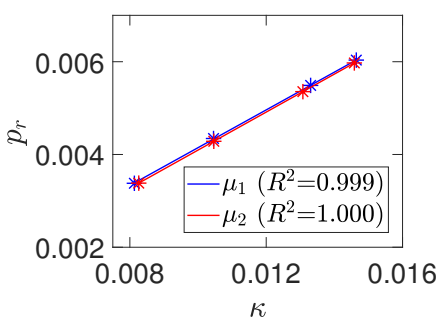
(39) Sb (t1)



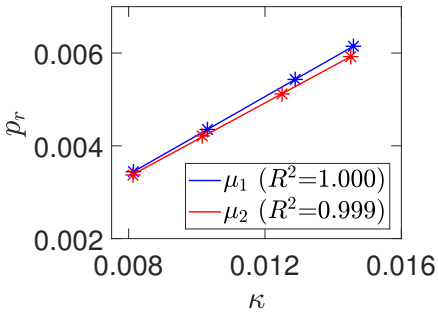
(40) GeSe



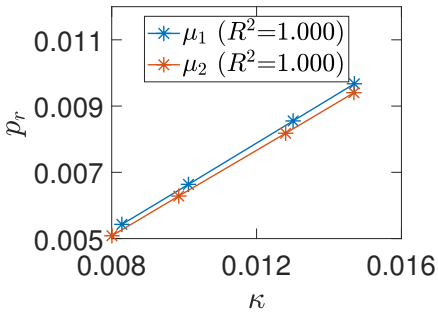
(41) GeS



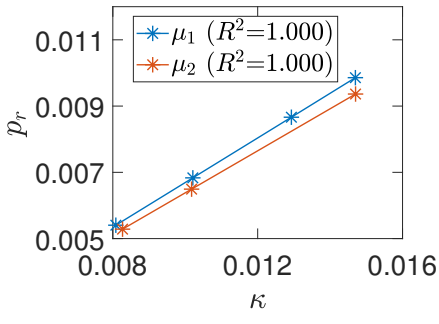
(42) SnSe



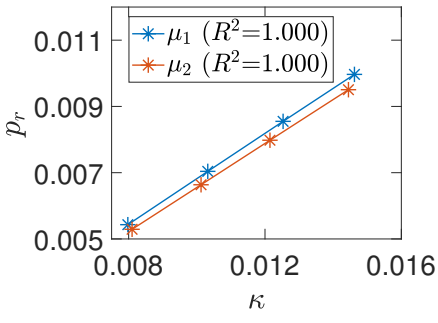
(43) SnS



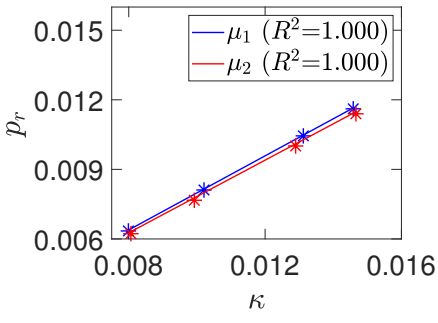
(44) ZrS_3



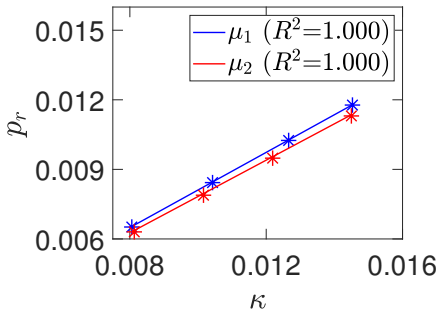
(45) TiS_3



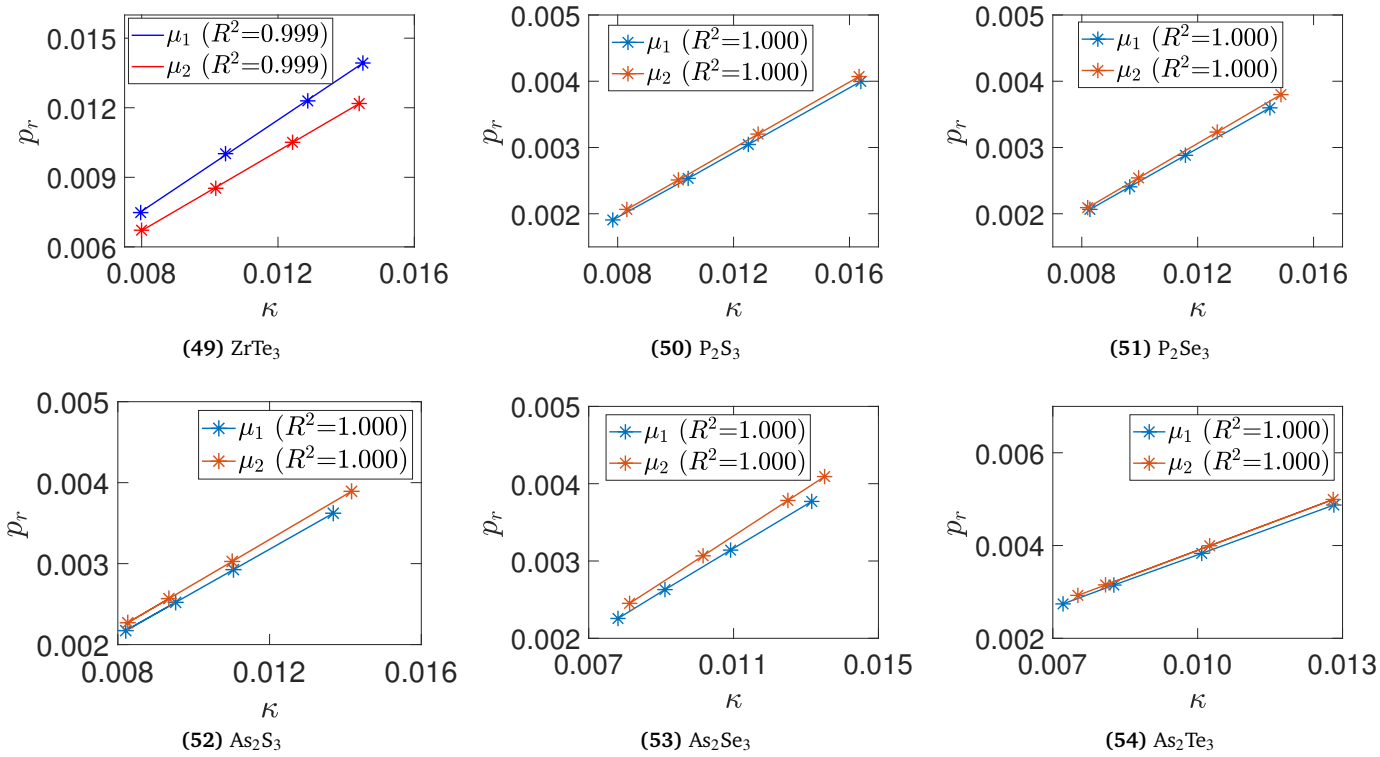
(46) $ZrSe_3$



(47) HfS_3



(48) $HfSe_3$



(49) $ZrTe_3$ **(50)** P_2S_3 **(51)** P_2Se_3

(52) As_2S_3 **(53)** As_2Se_3 **(54)** As_2Te_3

Figure 1 Radial polarization p_r (e/Bohr) as a function of the curvature κ (1/Bohr) for the fifty-four select atomic monolayers. The R^2 values in the legend denote the coefficient of determination for the linear regression. The mean R^2 value for all the plots taken together is 0.9987, verifying the quality of the linear fit.

Table 4 Representative results demonstrating the numerical accuracy of the transversal flexoelectric coefficients reported in this work. The superscript $(.)^*$ is used to denote values obtained when the real-space discretization as well as Brillouin-zone integration grid spacings are both refined by 66%, the relaxation tolerances are made 66% more stricter, and the vacuum is made 66% larger, all relative to those employed in this work.

Material	$\mu_1(e)$	$\mu_1^*(e)$	$\mu_2(e)$	$\mu_2^*(e)$
GaS (h1)	0.481	0.482	0.479	0.483
MoS_2 (h2)	0.577	0.579	0.576	0.578
C (h3)	0.216	0.213	0.217	0.214
P (h3)	0.248	0.244	0.252	0.256
SnS_2 (h4)	0.400	0.403	0.402	0.404
P (t1)	0.312	0.313	0.332	0.338
GeS (t1)	0.419	0.421	0.408	0.411
TiS_3 (t2)	0.673	0.679	0.634	0.628
As_2S_3 (t3)	0.272	0.274	0.279	0.283

Table 5 Flexoelectric coefficient relating polarization to bending moment, i.e., $\tilde{\mu} = \mu/D$, where D is the bending modulus, for the fifty-four select atomic monolayers from first principles DFT calculations.

Group	Material	$\tilde{\mu}_1$ (e/eV)	$\tilde{\mu}_2$ (e/eV)	Group	Material	$\tilde{\mu}_1$ (e/eV)	$\tilde{\mu}_2$ (e/eV)
Group III monochalcogenides (h1)	GaS	0.02	0.02	Group V monolayers (h3)	P	0.35	0.35
	GaSe	0.02	0.03		As	0.50	0.44
	InS	0.03	0.03		Bi	1.38	1.32
	InSe	0.03	0.03		Sb	1.17	1.09
	InTe	0.04	0.04	Group IV dichalcogenides (h4)	$GeSe_2$	0.10	0.09
	GaTe	0.04	0.04		GeS_2	0.10	0.07
Transition metal dichalcogenides (h2)	ZrS_2	0.73	0.56		$SnSe_2$	0.10	0.10
	TiS_2	0.17	0.18		SnS_2	0.13	0.13
	$ZrSe_2$	0.22	0.22	Group V monolayers (t1)	P	0.04	0.23
	$TiSe_2$	0.14	0.14		As	0.05	0.22
	NbS_2	0.10	0.10		Bi	0.14	0.49
	$NbSe_2$	0.11	0.10		Sb	0.14	0.47
	HfS_2	0.28	0.29	Group IV monochalcogenides (t1)	GeSe	0.10	0.29
	$ZrTe_2$	0.19	0.25		GeS	0.11	0.32
	$TiTe_2$	0.13	0.12		SnSe	0.09	0.18
	$MoSe_2$	0.06	0.06		SnS	0.10	0.17
	MoS_2	0.06	0.06	Transition metal trichalcogenides (t2)	ZrS_3	0.03	0.02
	WS_2	0.06	0.06		TiS_3	0.02	0.02
	WSe_2	0.05	0.05		$ZrSe_3$	0.02	0.02
	$NbTe_2$	0.11	0.13		HfS_3	0.03	0.03
	$MoTe_2$	0.06	0.07		$HfSe_3$	0.02	0.02
	WTe_2	0.06	0.06		$ZrTe_3$	0.04	0.01
Group IV, III-V monolayers (h3)	Si	0.53	0.51	Group V chalcogenides (t3)	P_2S_3	0.17	0.16
	BN	0.36	0.34		P_2Se_3	0.23	0.14
	C	0.15	0.15		As_2S_3	0.16	0.15
	Sn	3.71	3.12		As_2Se_3	0.18	0.16
	Ge	1.50	1.42		As_2Te_3	0.26	0.21

Table 6 Bending moduli along principal directions from first principles DFT calculations. D_1 and D_2 represent the bending moduli for bending along x_1 and x_2 directions, respectively. Values for the other materials can be found in Ref. [24]

Material	Bending moduli (eV) D_1	D_2	Material	Bending moduli (eV) D_1	D_2
GeS_2 (h4)	4.53	6.30	P_2S_3 (t3)	1.42	1.60
$GeSe_2$(h4)	4.38	4.73	P_2Se_3 (t3)	1.11	1.87
SnS_2 (h4)	3.32	3.34	As_2S_3 (t3)	1.70	1.90
$SnSe_2$ (h4)	4.07	3.99	As_2Se_3 (t3)	1.53	1.84
$ZrTe_3$ (t2)	24.5	76.2	As_2Te_3 (t3)	1.48	1.85

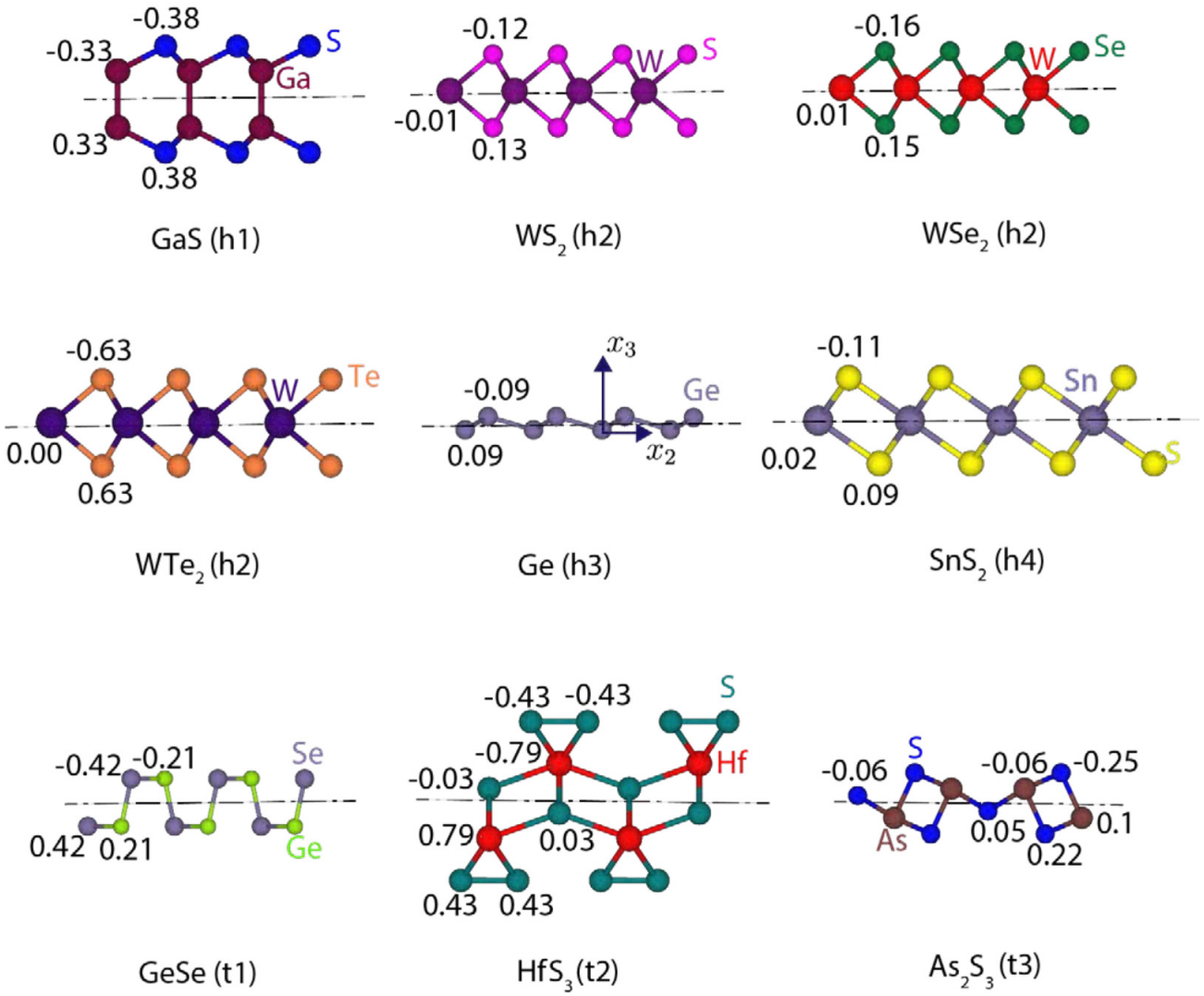


Figure 2 Charge transfer based on Bader analysis in representative atomic monolayers for bending along the x_1-direction at curvature $\kappa \sim 0.2$ nm^{-1}.

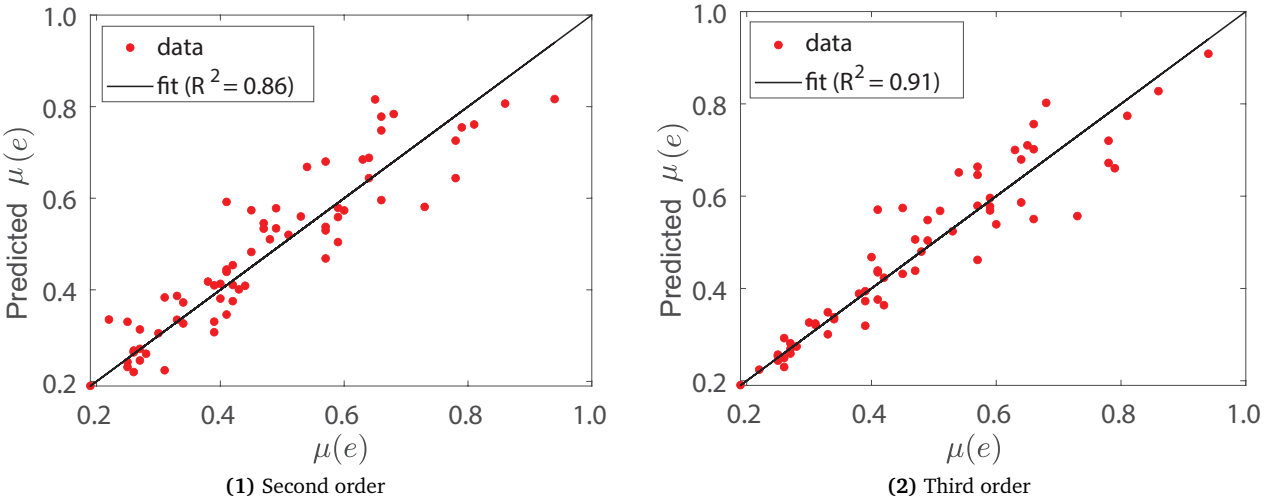


Figure 3 Set of calculated transversal flexoelectric coefficients and its polynomial regression with features being thickness, elastic modulus along the bending direction, and the sum of polarizability of constituent atoms.