Electronic supplementary information (ESI)

Ab-initio study on the two-dimensional anisotropic monolayers ScXY (X =S, Se; Y = Cl, Br) for the photocatalytic water splitting applications with high carrier mobilities

Fei-Yang Xu [1], Yu Zhou [2], Tian Zhang [3], Zhao-Yi Zeng [4,*], Xiang-Rong Chen [1,*], Hua-Yun Geng [5]

[1] Institute of Atomic and Molecular Physics, College of Physics, Sichuan University, Chengdu 610065, China

[2] Department of Physics, College of Basic Medical Sciences, Army Medical University, Chongqing 400038, China

[3] College of Physics and Electronic Engineering, Sichuan Normal University, Chengdu 610101, China

[4] College of Physics and Electronic Engineering, Chongqing Normal University, Chongqing 400047, China

[5] National Key Laboratory for Shock Wave and Detonation Physics Research, Institute of Fluid Physics, CAEP, Mianyang 621900, China

[*] *Corresponding authors. E-mail*: zhaoyizeng@cqnu.edu.cn; xrchen@scu.edu.cn

Table S1. The calculated linear elastic constants of the ScXY monolayers

Material	C_{11}	C_{12}	C_{22}	C_{66}
ScSCl	90.843	12.574	71.150	20.896
ScSBr	86.886	12.602	66.654	20.822
ScSeCl	84.166	10.652	64.543	18.307
ScSeBr	80.449	10.063	60.441	18.024

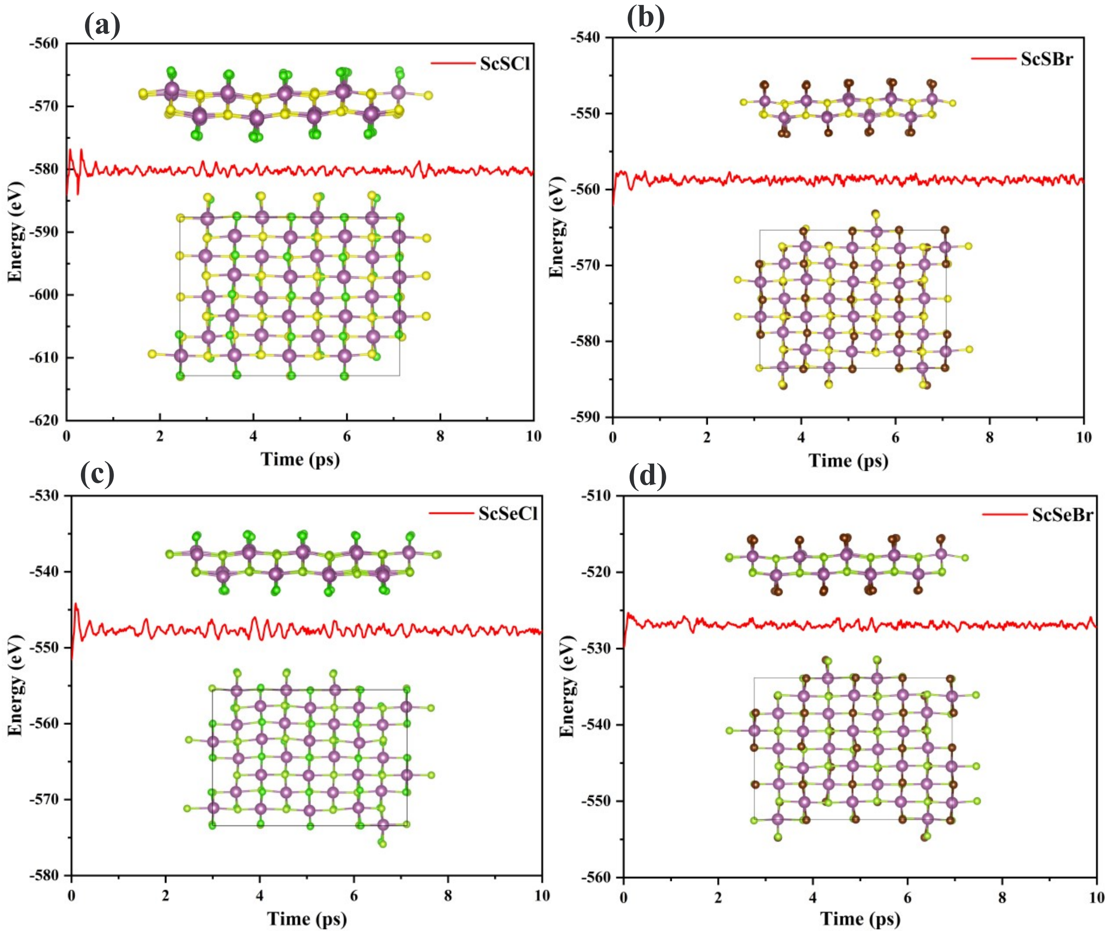
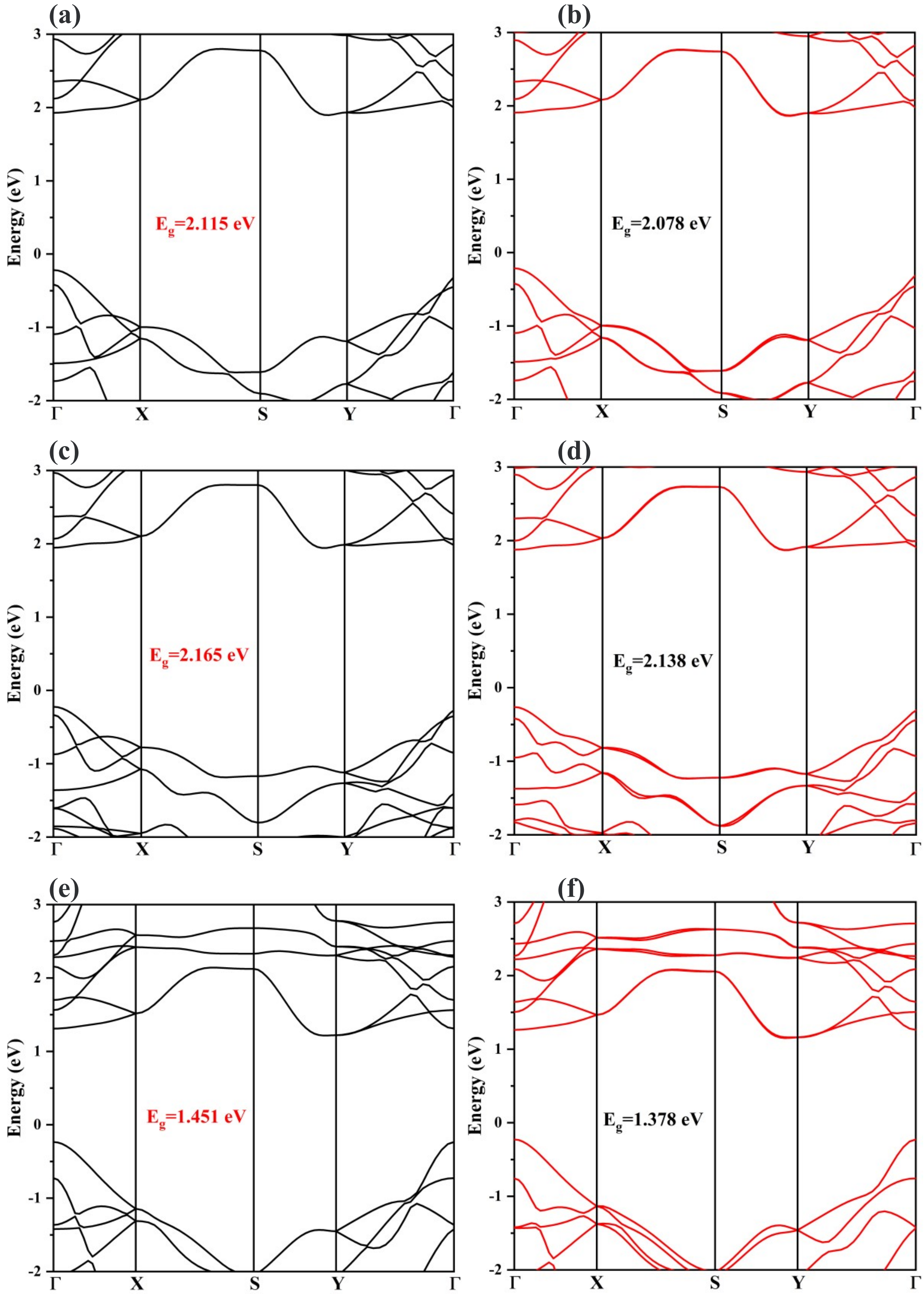


Fig. S1. The energy fluctuation of ScSCl (a), ScSBr (b), ScSeCl (c), and ScSeBr (d) monolayers throughout the simulation. A 4 × 4 × 1 supercell was selected to carry out the AIMD simulation, no enormous fluctuations are found in energy at 300 K, suggesting that these four monolayers are thermally stable.


(a)
E$_g$=2.115 eV
(b)
E$_g$=2.078 eV
(c)
E$_g$=2.165 eV
(d)
E$_g$=2.138 eV
(e)
E$_g$=1.451 eV
(f)
E$_g$=1.378 eV
Energy (eV)
Γ
X
S
Y
Γ

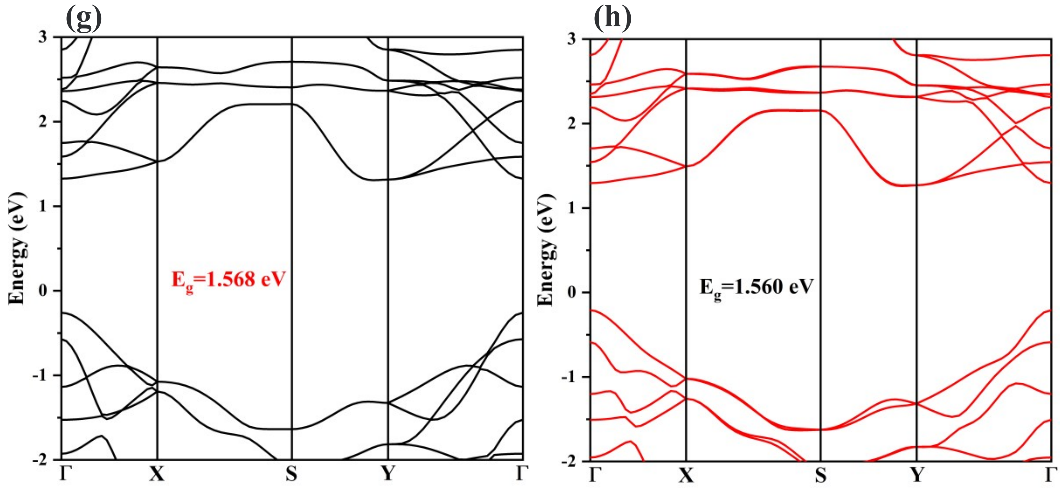


Fig. S2. The band structure of the ScXY (X=S, Se; Y=Cl, Br) monolayers calculated from the PBE level. (a, c, e, g) is obtained from pure PBE for monolayer ScSCl, ScSBr, ScSeCl, and ScSeBr, respectively, and (b, d, f, h) is the corresponding result from PBE with SOC.

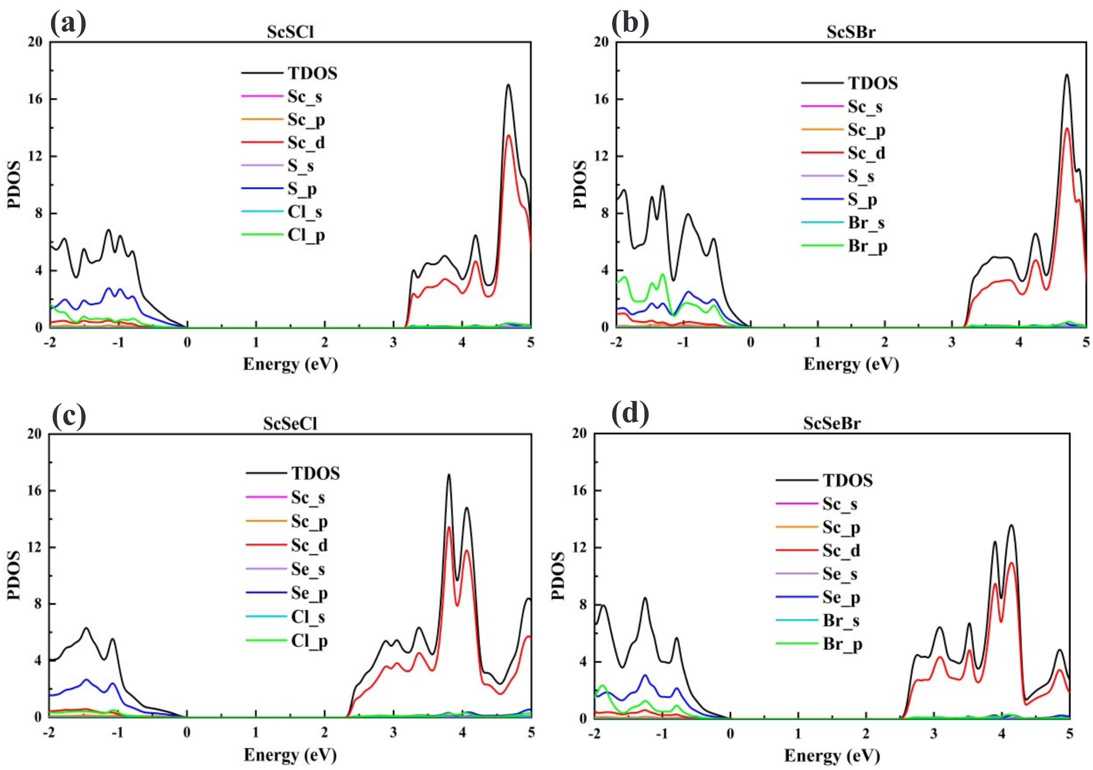


Fig. S3. The calculated partial density of state of ScSCl (a), ScSBr (b), ScSeCl (c), and ScSeBr (d) monolayers at the HSE06 level.

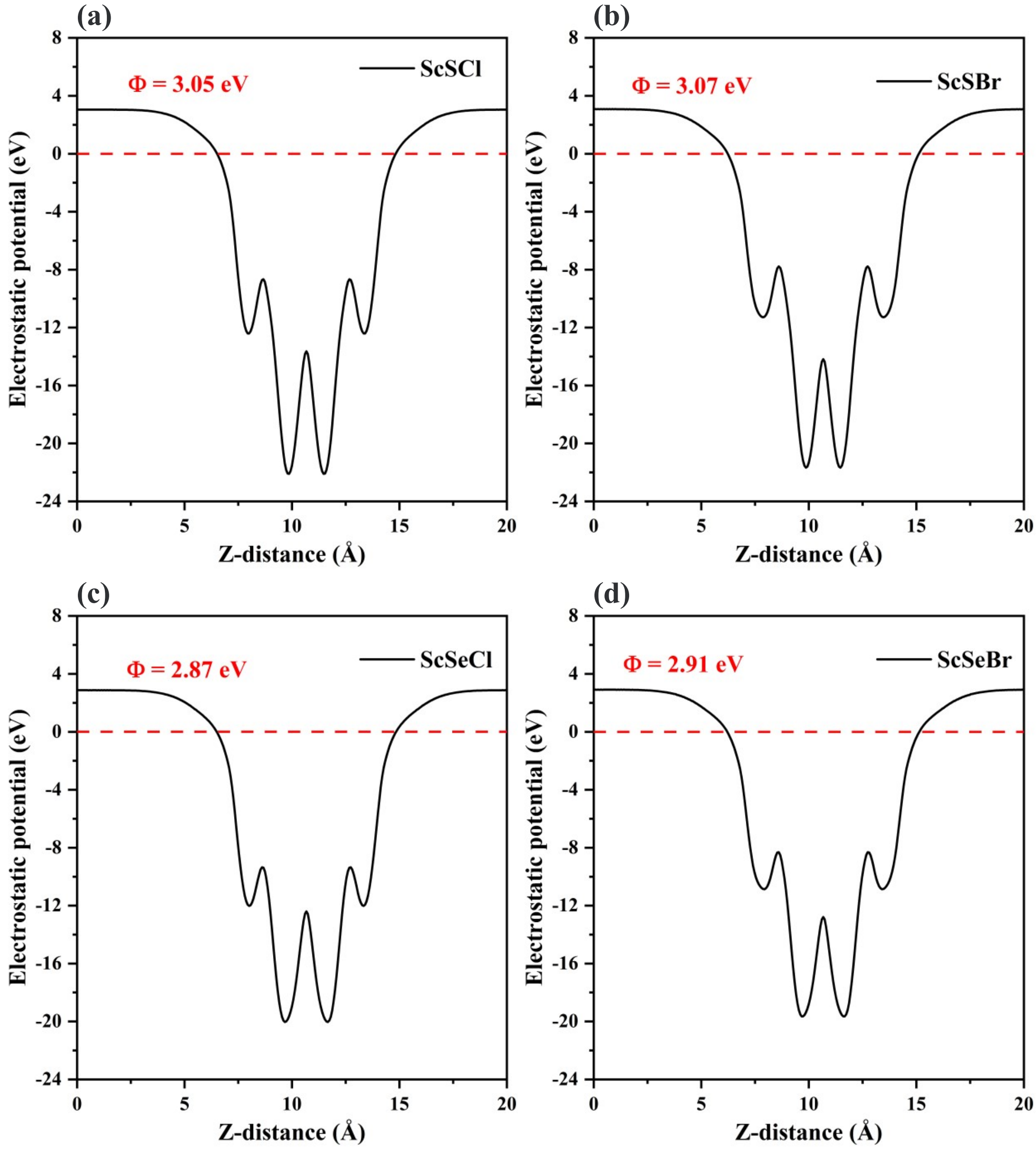


Fig. S4. The calculated average electrostatic potential for ScSCl (a), ScSBr (b), ScSeCl (c), and ScSeBr (d) monolayers with HSE06 functional.

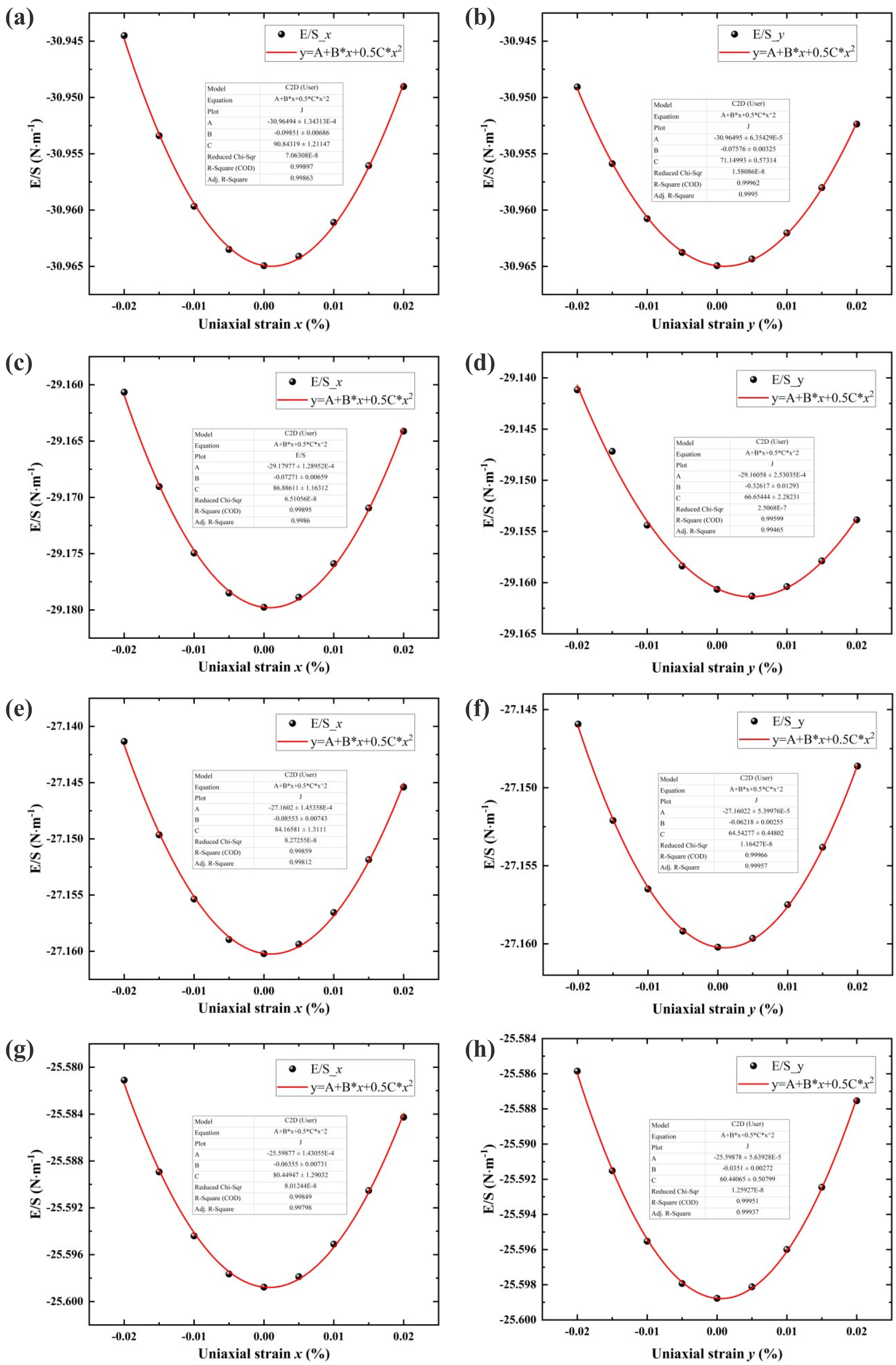
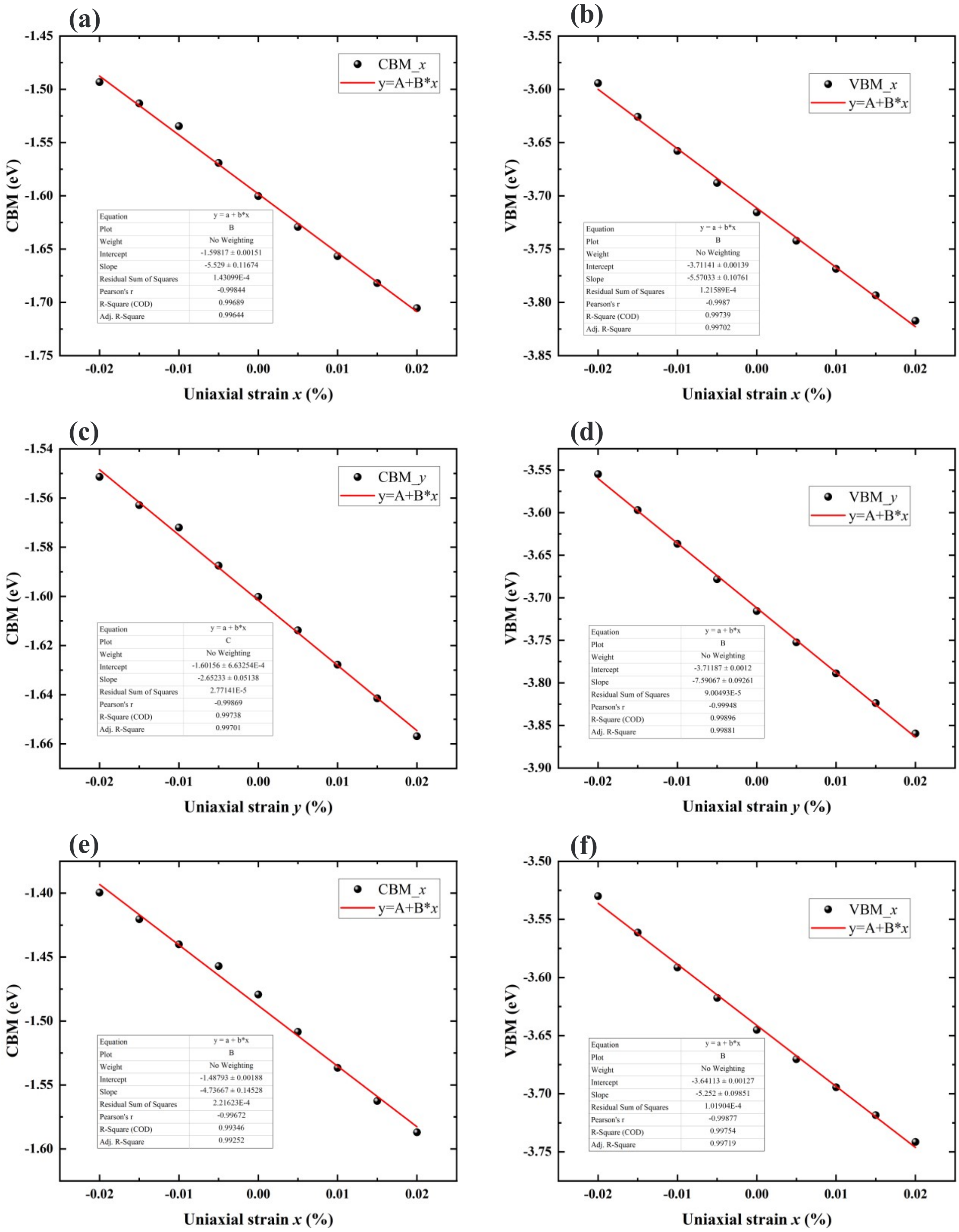


Fig. S5. The elastic modulus C_{2D} along the propagation direction is obtained through the quadratic function fitting the total energy of the system under strain for monolayer ScSCl in the (a) *x*- and (b) *y*-directions; for monolayer ScSBr in the (c) *x*- and (d) *y*-directions; for monolayer ScSeCl in the (e) *x*- and (f) *y*-directions; for monolayer ScSeBr in the (g) *x*- and (h) *y*-directions.


(a)
CBM_x
y=A+B*x
CBM (eV)
Uniaxial strain x (%)
Equation y = a + b*x
Plot B
Weight No Weighting
Intercept -1.59817 ± 0.00151
Slope -5.529 ± 0.11674
Residual Sum of Squares 1.43099E-4
Pearson's r -0.99844
R-Square (COD) 0.99689
Adj. R-Square 0.99644
(b)
VBM_x
y=A+B*x
VBM (eV)
Uniaxial strain x (%)
Equation y = a + b*x
Plot B
Weight No Weighting
Intercept -3.71141 ± 0.00139
Slope -5.57033 ± 0.10761
Residual Sum of Squares 1.21589E-4
Pearson's r -0.9987
R-Square (COD) 0.99739
Adj. R-Square 0.99702
(c)
CBM_y
y=A+B*x
CBM (eV)
Uniaxial strain y (%)
Equation y = a + b*x
Plot C
Weight No Weighting
Intercept -1.60156 ± 6.63254E-4
Slope -2.65233 ± 0.05138
Residual Sum of Squares 2.77141E-5
Pearson's r -0.99869
R-Square (COD) 0.99738
Adj. R-Square 0.99701
(d)
VBM_y
y=A+B*x
VBM (eV)
Uniaxial strain y (%)
Equation y = a + b*x
Plot B
Weight No Weighting
Intercept -3.71187 ± 0.0012
Slope -7.59067 ± 0.09261
Residual Sum of Squares 9.00493E-5
Pearson's r -0.99948
R-Square (COD) 0.99896
Adj. R-Square 0.99881
(e)
CBM_x
y=A+B*x
CBM (eV)
Uniaxial strain x (%)
Equation y = a + b*x
Plot B
Weight No Weighting
Intercept -1.48793 ± 0.00188
Slope -4.73667 ± 0.14528
Residual Sum of Squares 2.21623E-4
Pearson's r -0.99672
R-Square (COD) 0.99346
Adj. R-Square 0.99252
(f)
VBM_x
y=A+B*x
VBM (eV)
Uniaxial strain x (%)
Equation y = a + b*x
Plot B
Weight No Weighting
Intercept -3.64113 ± 0.00127
Slope -5.252 ± 0.09851
Residual Sum of Squares 1.01904E-4
Pearson's r -0.99877
R-Square (COD) 0.99754
Adj. R-Square 0.99719

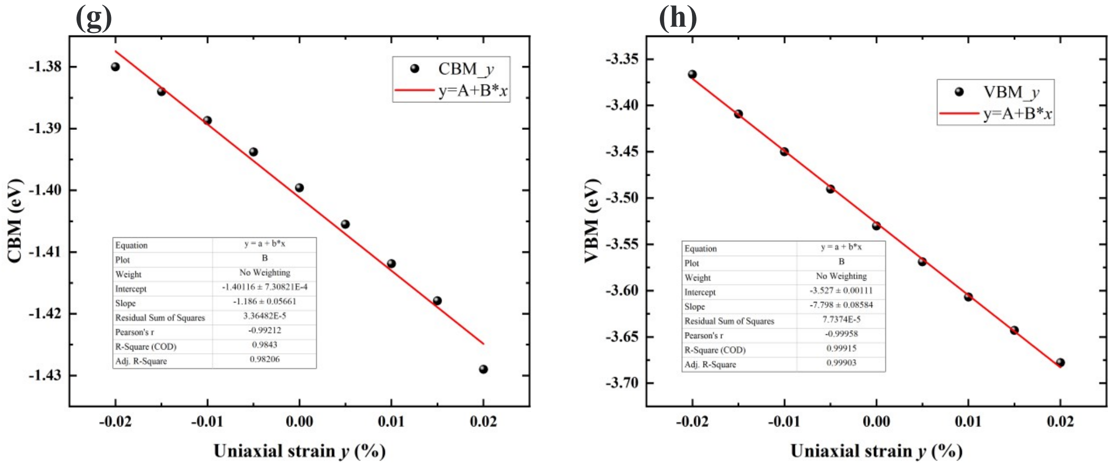


Fig. S6. Fitting the elastic modulus constant E_l for monolayer ScSCl: (a) *x*-axis uniaxial strained CBM, (b) *x*-axis uniaxial strained VBM, (c) *y*-axis uniaxial strained CBM and (d) *y*-axis uniaxial strained VBM; for monolayer ScSBr: (e) *x*-axis uniaxial strained CBM, (f) *x*-axis uniaxial strained VBM, (g) *y*-axis uniaxial strained CBM and (h) *y*-axis uniaxial strained VBM.

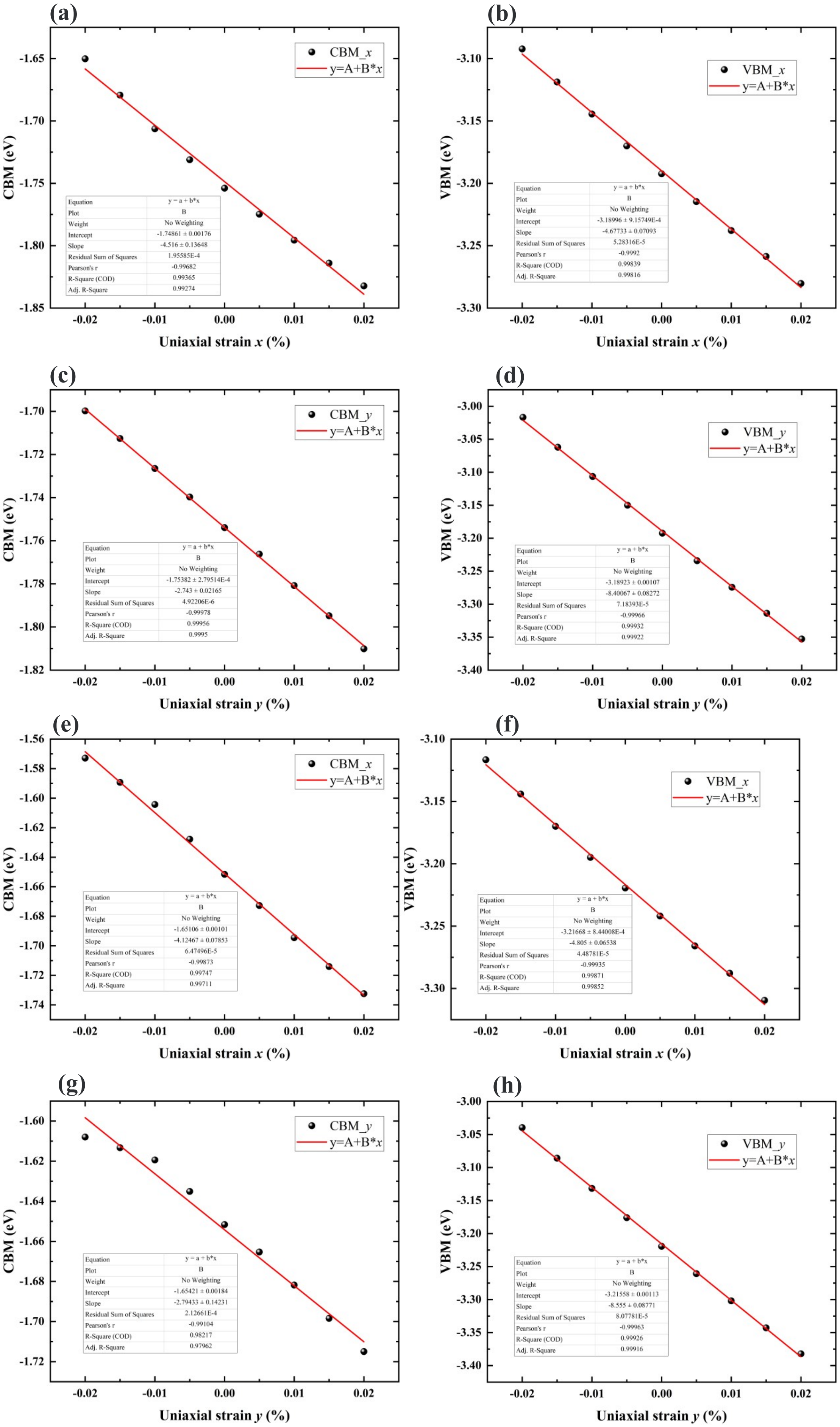

(a)
CBM_x
y=A+B*x
Equation y = a + b*x
Plot B
Weight No Weighting
Intercept -1.74861 ± 0.00176
Slope -4.516 ± 0.13648
Residual Sum of Squares 1.95585E-4
Pearson's r -0.99682
R-Square (COD) 0.99365
Adj. R-Square 0.99274
CBM (eV)
Uniaxial strain x (%)
(b)
VBM_x
y=A+B*x
Equation y = a + b*x
Plot B
Weight No Weighting
Intercept -3.18996 ± 9.15749E-4
Slope -4.67733 ± 0.07093
Residual Sum of Squares 5.28316E-5
Pearson's r -0.9992
R-Square (COD) 0.99839
Adj. R-Square 0.99816
VBM (eV)
Uniaxial strain x (%)
(c)
CBM_y
y=A+B*x
Equation y = a + b*x
Plot B
Weight No Weighting
Intercept -1.75382 ± 2.79514E-4
Slope -2.743 ± 0.02165
Residual Sum of Squares 4.92206E-6
Pearson's r -0.99978
R-Square (COD) 0.99956
Adj. R-Square 0.9995
CBM (eV)
Uniaxial strain y (%)
(d)
VBM_y
y=A+B*x
Equation y = a + b*x
Plot B
Weight No Weighting
Intercept -3.18923 ± 0.00107
Slope -8.40067 ± 0.08272
Residual Sum of Squares 7.18393E-5
Pearson's r -0.99966
R-Square (COD) 0.99932
Adj. R-Square 0.99922
VBM (eV)
Uniaxial strain y (%)
(e)
CBM_x
y=A+B*x
Equation y = a + b*x
Plot B
Weight No Weighting
Intercept -1.65106 ± 0.00101
Slope -4.12467 ± 0.07853
Residual Sum of Squares 6.47496E-5
Pearson's r -0.99873
R-Square (COD) 0.99747
Adj. R-Square 0.99711
CBM (eV)
Uniaxial strain x (%)
(f)
VBM_x
y=A+B*x
Equation y = a + b*x
Plot B
Weight No Weighting
Intercept -3.21668 ± 8.44008E-4
Slope -4.805 ± 0.06538
Residual Sum of Squares 4.48781E-5
Pearson's r -0.99935
R-Square (COD) 0.99871
Adj. R-Square 0.99852
VBM (eV)
Uniaxial strain x (%)
(g)
CBM_y
y=A+B*x
Equation y = a + b*x
Plot B
Weight No Weighting
Intercept -1.65421 ± 0.00184
Slope -2.79433 ± 0.14231
Residual Sum of Squares 2.12661E-4
Pearson's r -0.99104
R-Square (COD) 0.98217
Adj. R-Square 0.97962
CBM (eV)
Uniaxial strain y (%)
(h)
VBM_y
y=A+B*x
Equation y = a + b*x
Plot B
Weight No Weighting
Intercept -3.21558 ± 0.00113
Slope -8.555 ± 0.08771
Residual Sum of Squares 8.07781E-5
Pearson's r -0.99963
R-Square (COD) 0.99926
Adj. R-Square 0.99916
VBM (eV)
Uniaxial strain y (%)

Fig S7. Fitting the elastic modulus constant E_l for monolayer ScSeCl: (a) *x*-axis uniaxial strained CBM, (b) *x*-axis uniaxial strained VBM, (c) *y*-axis uniaxial strained CBM and (d) *y*-axis uniaxial strained VBM; for monolayer ScSeBr: (e) *x*-axis uniaxial strained CBM, (f) *x*-axis uniaxial strained VBM, (g) *y*-axis uniaxial strained CBM and (h) *y*-axis uniaxial strained VBM.