Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information

Electromechanical response of group-IV monochalcogenide monolayers

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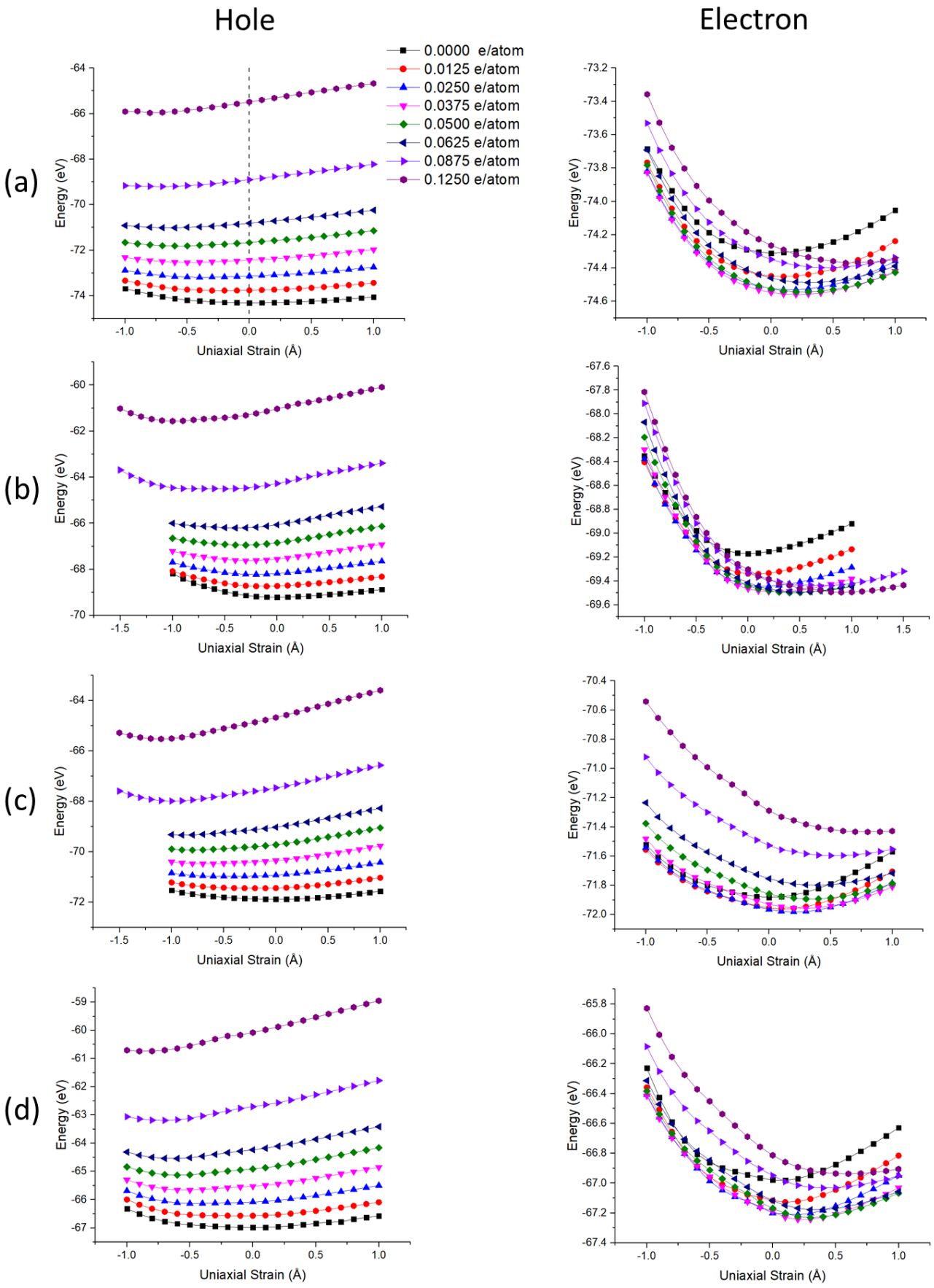
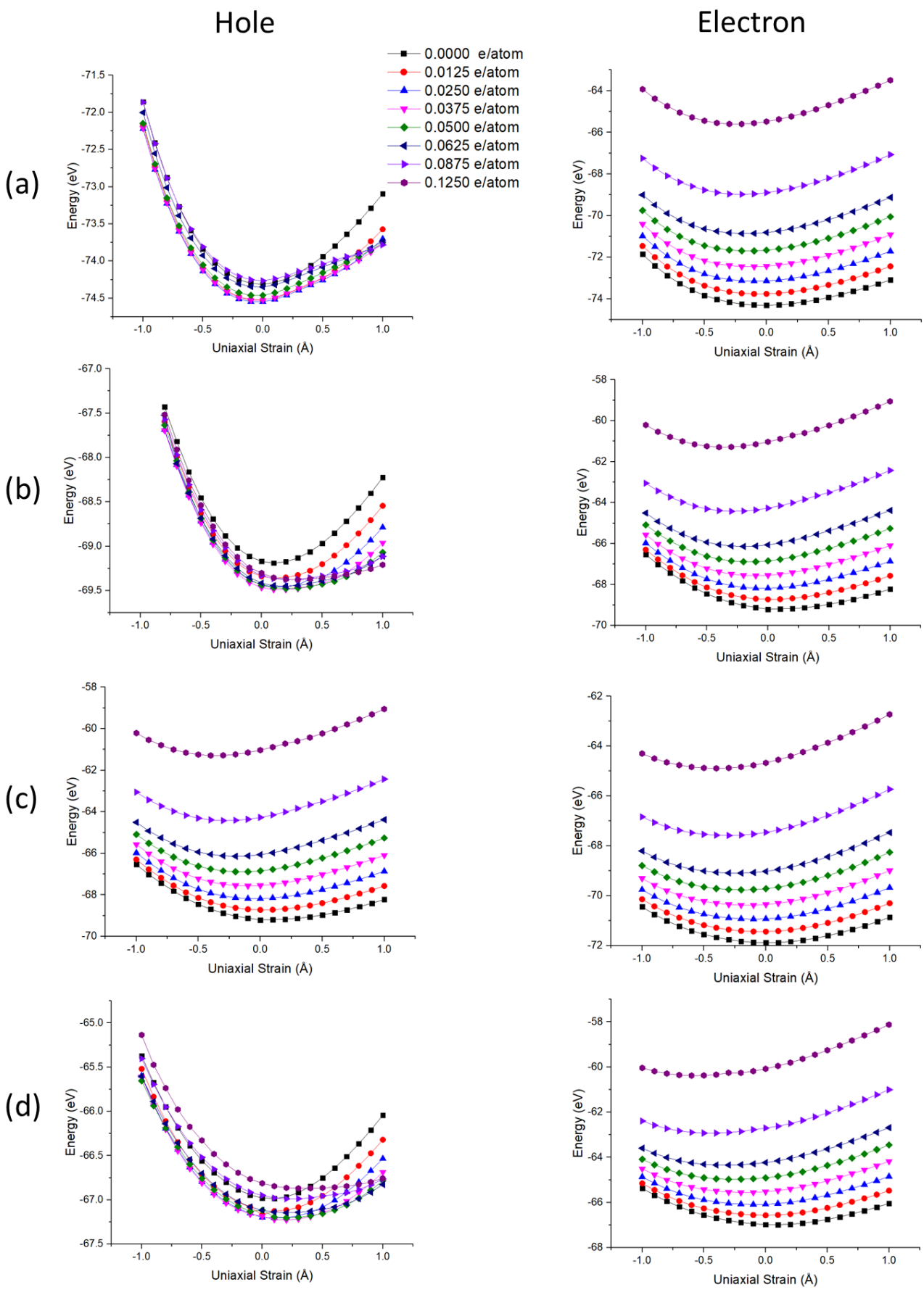
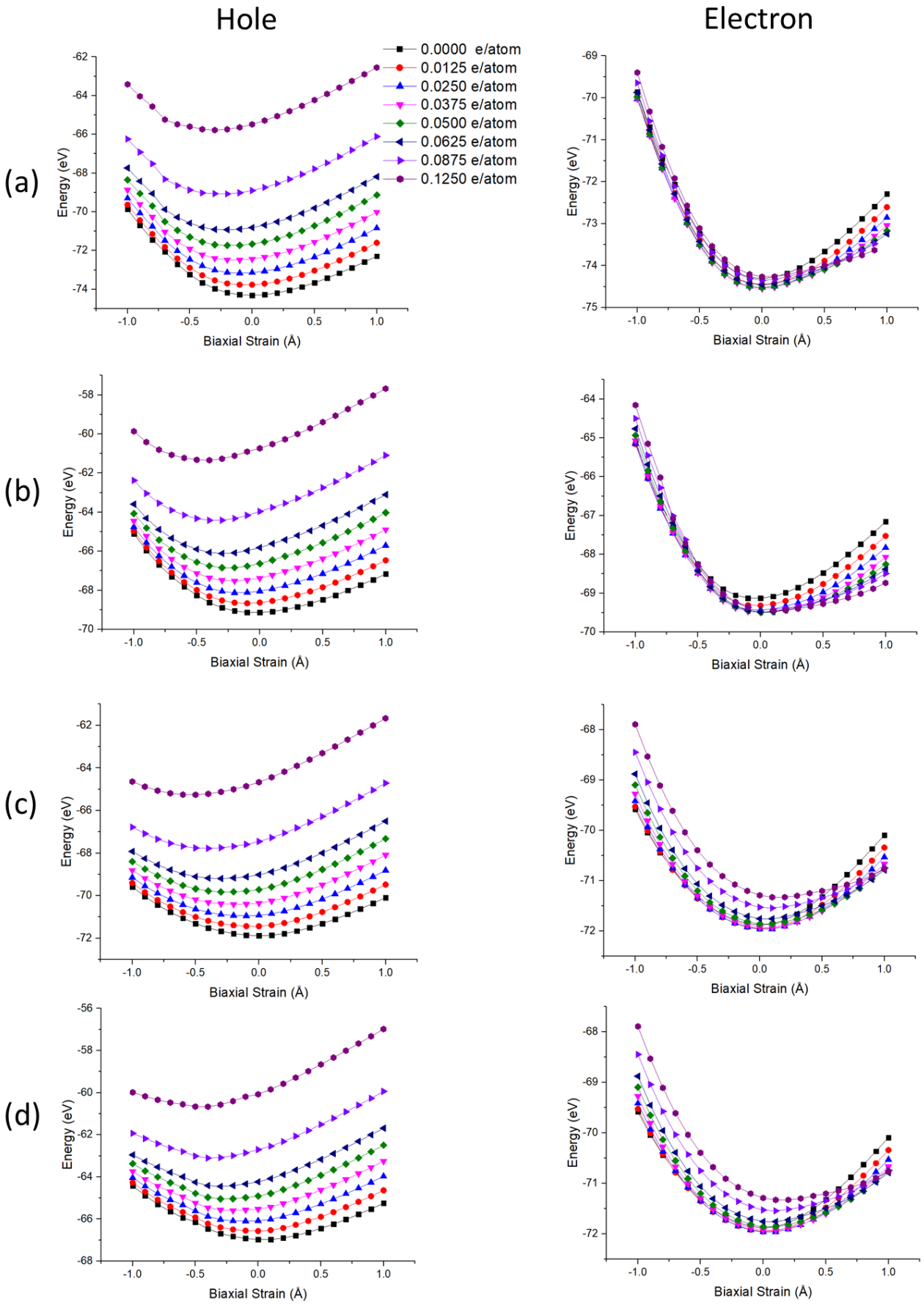


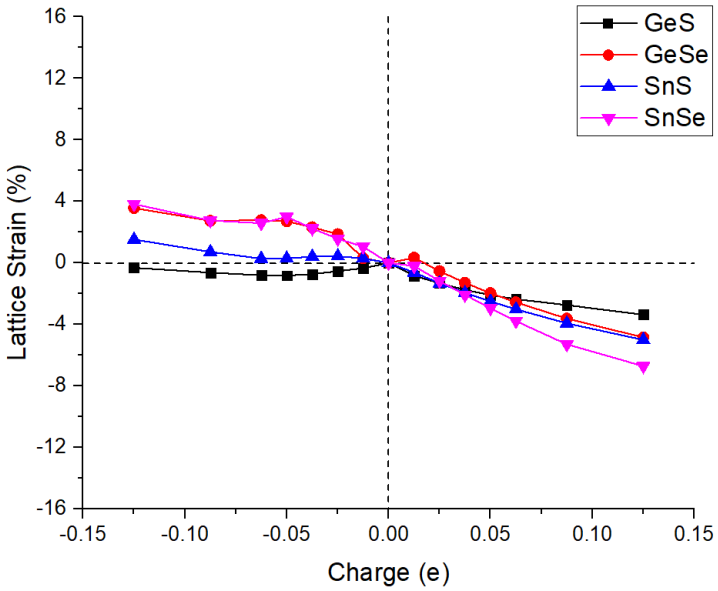
Supplementary Figure 1: Total energy of (a) GeS, (b) GeSe, (c) SnS and (d) SnSe monolayers as a function of strain applied on lattice parameter *b* and injected hole and electron



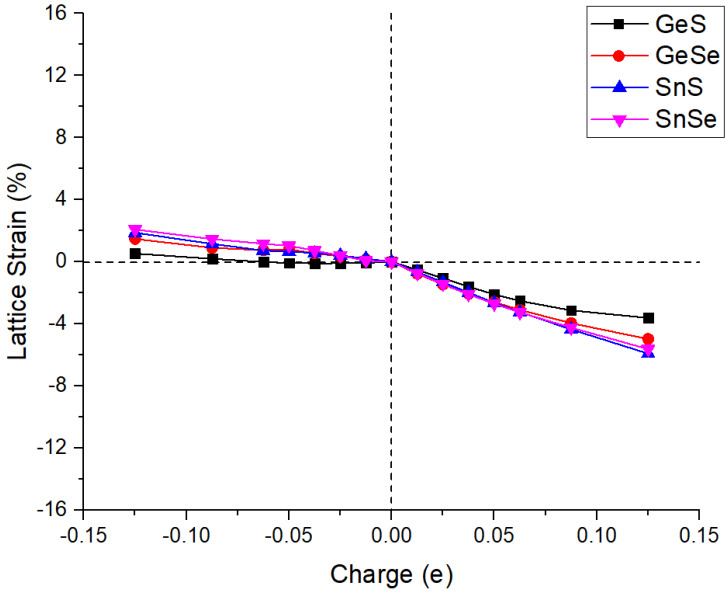
Supplementary Figure 2: Total energy of (a) GeS, (b) GeSe, (c) SnS and (d) SnSe monolayers as a function of strain applied on lattice parameter *a* and injected hole and electron



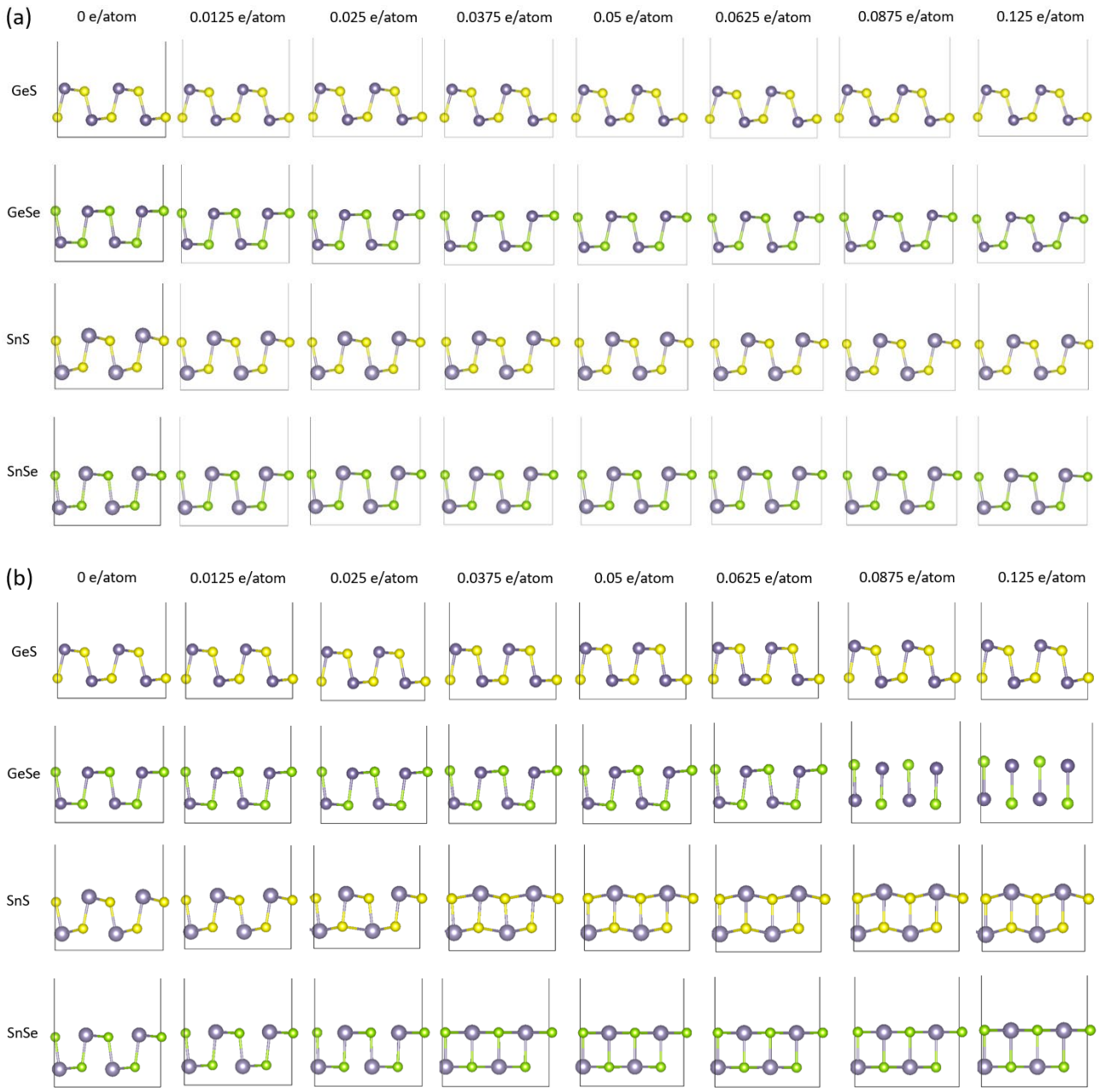
Supplementary Figure 3: Total energy of (a) GeS, (b) GeSe, (c) SnS and (d) SnSe monolayers as a function of strain applied on lattice parameter *a* and *b* and injected hole and elecron



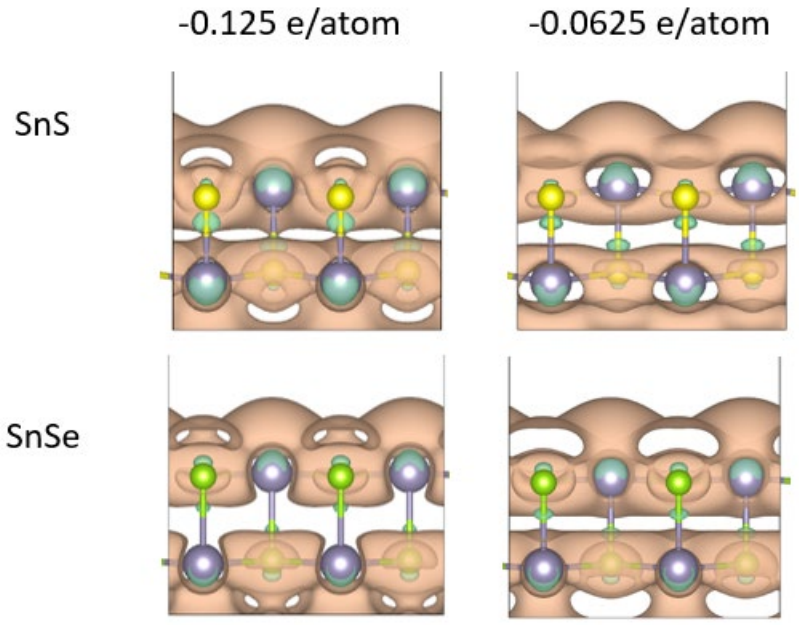
Supplementary Figure 4: Electromechanical strain responses of group IV monochalcogenides along the zig-zag direction, upon electron (negative) and hole (positive) injection.



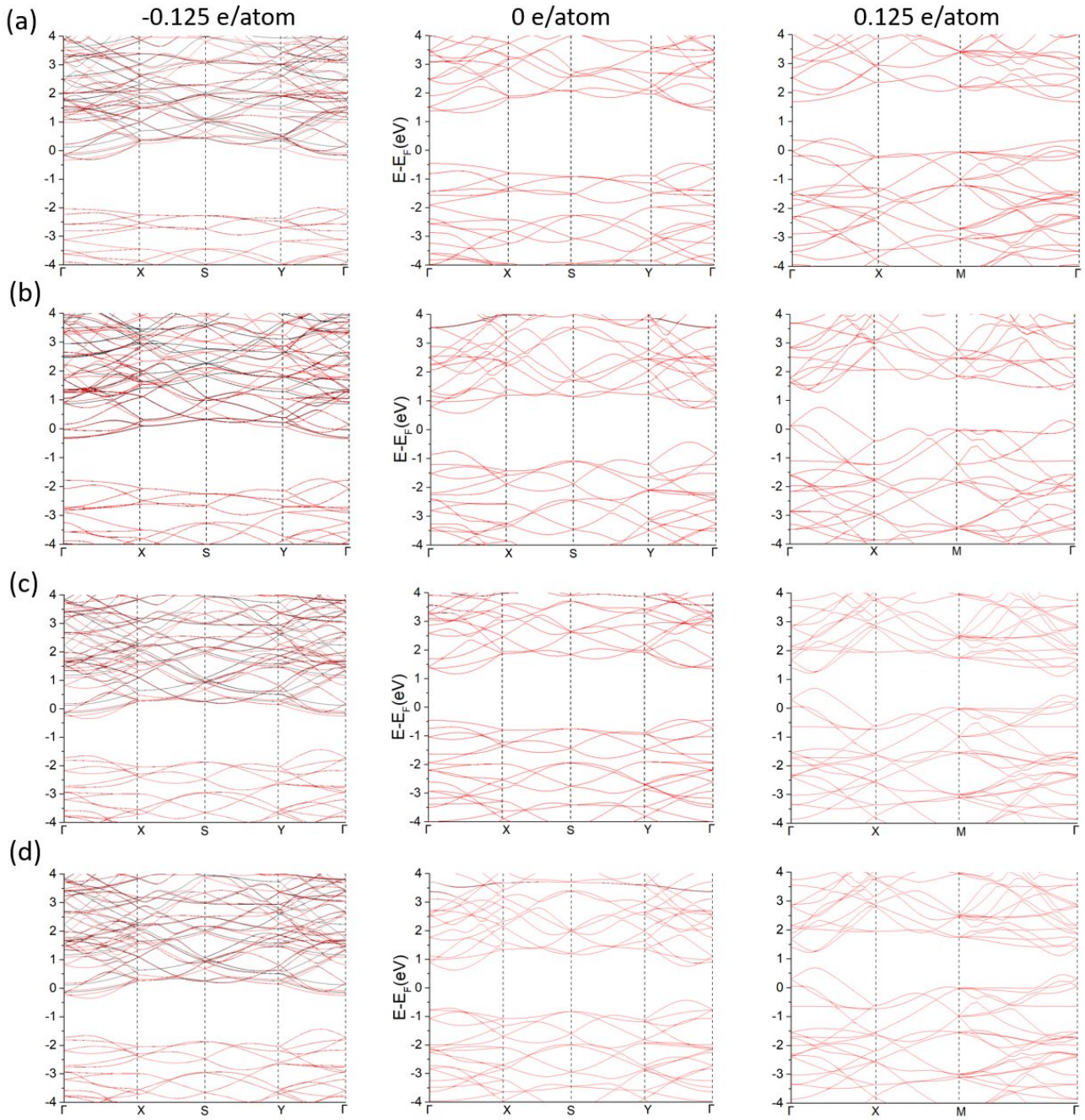
Supplementary Figure 5: Electromechanical strain responses of group IV monochalcogenides along both armchair and zig-zag directions, upon electron (negative) and hole (positive) injection.



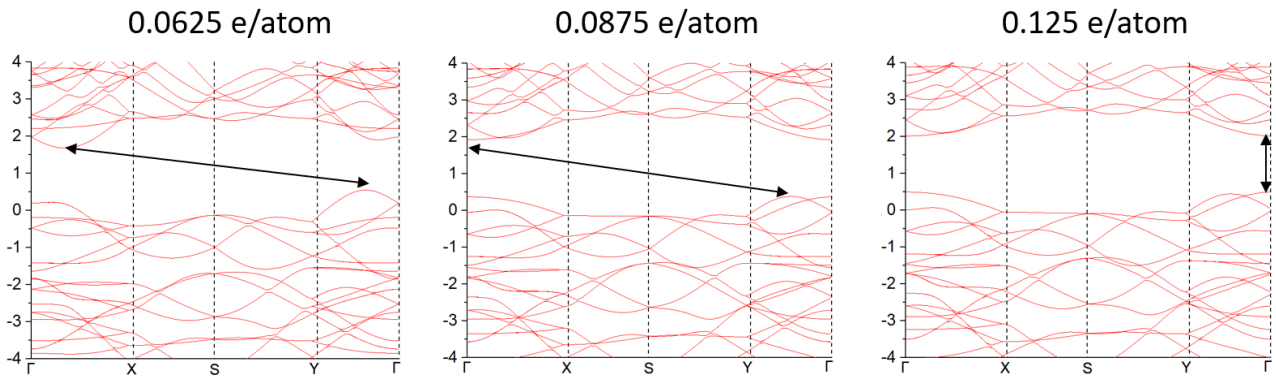
Supplementary Figure 6: Armchair view of the evolution of the group-IV monochalcogenide monolayers upon (a) electron and (b) hole injection.



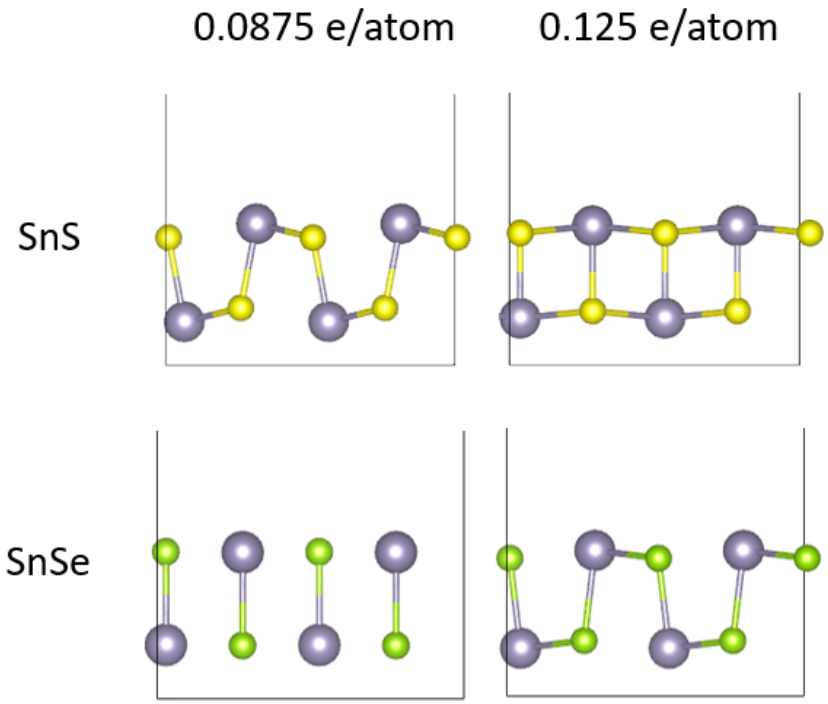
Supplementary Figure 7. Zig-zag views of charge density distribution: Charge density distribution of the SnS and SnSe monolayer upon charge injection at iso-surface values of 0.0003 and 0.0006 e/Bohr^3. Excess electron and hole are represented by the orange and green colours respectively.



Supplementary Figure 8: (a-d) Band structures of GeS, GeSe, SnS and SnSe monolayers upon charge injection. The black and red lines represent spin up and spin down states, respectively.



Supplementary Figure 9: Band structures of GeS monolayer upon hole injection. The black arrows represent the band gap.



Supplementary Figure 10: Armchair view of the optimised group-IV monochalcogenide monolayers upon hole injection with fixed in-plane charge-neutral lattice constants

Supplementary Table 1: Elastic constants, C_{11} and C_{22}, of monolayer group-IV monochalcogenides and phosphorene.

	C_{11} (armchair) N/m	C_{22} (Zigzag) N/m
GeS	13.6	44.0
GeSe	14.3	46.9
SnS	15.2	37.2
SnSe	20.0	41.4
Phosphorene[1]	21.7	89.9

References:

1. Wu, B.; Deng, H.-X.; Jia, X.; Shui, L.; Gao, E.; Liu, Z., High-performance phosphorene electromechanical actuators. *npj Computational Materials* **2020,** *6* (1).