

List of Figures

- Figure 1.1:** Representative scheme for electrical energy harvesting from green energy and excessive electricity storage, conversion, and utilization. Reproduced from [13] 4
- Figure 2.1:** Schematic representation of first HK theorem. Here, the HK theorem completes the circle, while other smaller arrow shows the solution of Schrödinger equation. Image adapted from ref. [18] 32
- Figure 2.2:** Same as Figure 2.1 but for Kohn-Sham ansatz. HK_0 defines Hohenberg and Kohn theorem applied to non-interacting system. The connection between many-body and the independent particle systems provided by Kohn-Sham that labelled as double arrow. Image is adapted from ref. [21] 34
- Figure 2.3:** Schematic flowchart for finding self-consistent solutions of the Kohn-Sham equations. [From Quantum Espresso Tutorial] 37
- Figure 2.4:** Comparison of wavefunction in Coulomb potential of nucleus (blue) and pseudopotential (red) inside and outside the cutoff region. Pseudo and real wavefunctions match after the cutoff radius. Image is adapted from ref. [21] 42
- Figure 3.1:** Top and side views of optimised geometries of (a) pristine SnSe₂ and (b) doped-SnSe₂. [4] 54
- Figure 3.2:** The DOS of (a) pristine SnSe₂, (b) Na-doped SnSe₂, (c) K- doped SnSe₂ and (d) Ca-doped SnSe₂. [4] 55
- Figure 3.3:** Top and side view of (a) hydrogen adsorbed and (b) oxygen adsorbed doped-SnSe₂. [4] 56
- Figure 3.4:** PDOS of hydrogen adsorbed on (a) SnSe₂ and doped ((b) Na, (c) K and (d) Ca)) SnSe₂ monolayer. [4] 57
- Figure 3.5:** PDOS of oxygen adsorbed on (a) SnSe₂ and doped ((b) Na, (c) Ca and (d) K)) SnSe₂ monolayer. [4] 59
- Figure 3.6:** Plot for photon energy (a) pristine SnSe₂, (b) Na, (c) Ca and (d) K-doped SnSe₂ monolayers. [4] 63
- Figure 3.7:** Work function of (a) pristine SnSe₂ and ((b) Na, (c) K and (d) Ca) doped-SnSe₂ monolayers. [4] 63

Figure 3.8: Reaction coordinate (a) HER and (b) OER of pristine SnSe ₂ and doped-SnSe ₂ monolayers. [4]	64
Figure 4.1: Optimized geometries of (a) pristine (b) V _{se} defected, (b) V _{Se₂} defected, (c) V _{SnSe₃} defected and (d) V _{SnSe₆} defected SnSe ₂ monolayers.	76
Figure 4.2: The most stable adsorption site for H adsorption on (a) pristine and (b) V _{se} , (c) V _{Se₂} , (d) V _{SnSe₃} and (e) V _{SnSe₆} defected SnSe ₂ monolayers.	77
Figure 4.3: PDOS of (a) pristine SnSe ₂ and (b) H-adsorbed pristine SnSe ₂ monolayer.	79
Figure 4.4: PDOS of (a) V _{se} defect and H-adsorption on hollow site and (b) V _{Se₂} defect and H-adsorption on Se site.	80
Figure 4.5: PDOS of (a) V _{SnSe₃} defect and H-adsorption on hollow site and (b) V _{SnSe₆} defect and H-adsorption on hollow site.	81
Figure 4.6: Reaction coordinate of HER activity for pristine and defected SnSe ₂ monolayer.	84
Figure 5.1: The optimized geometries of (a) HfS ₂ , (b) HfSe ₂ and (c) HfSSe monolayers.	99
Figure 5.2: Band structure of pristine (a) HfS ₂ , (b) HfSe ₂ and (c) HfSSe monolayers.	100
Figure 5.3: The optimized geometries of H-adsorbed (a) HfS ₂ , (b) HfSe ₂ and (c) HfSSe monolayers.	101
Figure 5.4: PDOS of pristine (a) HfS ₂ , (b) HfSe ₂ and (c) HfSSe monolayers.	103
Figure 5.5: The optimized structure of various defect engineered (a) HfS ₂ , (b) HfSe ₂ and (c) HfSSe monolayers.	104
Figure 5.6: The optimized structures of H-adsorption on various defect engineered (a) HfS ₂ , (b) HfSe ₂ and (c) HfSSe monolayers.	105
Figure 5.7: PDOS of H-adsorption over the defect engineered (a) HfS ₂ , (b) HfSe ₂ and (c) HfSSe monolayers.	107
Figure 5.8: Comparison of ΔG^H of various TMDs in volcano plot for HER.	108