

## List of Figures

Figure Number	Figure Caption	Page Number
1.1	Schematic depicts the different classes of ultrathin 2D materials along with electronic, mechanical and dynamical properties of graphene at centre. Reproduced from Ref. 23.	3
1.2	Growth of research papers based on two-dimensional materials. (From web of science data <a href="http://www.webofknowledge.com">www.webofknowledge.com</a> ).	5
1.3	Schematic of 2D materials by reducing dimension along the z direction and xy directions.	7
1.4	Schematic of tuning 2D TMD properties by constructing hetero-structures.	11
1.5	Schematic of 2D hetero-structure with ion or molecules intercalation.	12
2.1	Schematic representation of first Hohenberg and Kohn theorem. Here, the HK theorem completes the circle, while arrow shows the solution of Schrödinger equation.	35
2.2	The connection between many body and the independent particle system is provided by Kohn – Sham, where $HK_0$ defines Hohenberg and Kohn theorem applied to non-interacting system	37
3.1	(a) Top and side view of optimized geometric structure of buckled arsenene (b) electronic bands structure of arsenene using PBE exchange-correlation function.	60
3.2	(a) Top and side view of functionalized arsenene, purple sphere as dopants (B, N, O, Ga, Ge and Se) and sky-blue sphere one As. (b) Cyan sphere is hydrogen adsorbed on dopant atoms. (c) Red one sphere is oxygen adsorbed on dopant atoms	62
3.3	The band structure of the B, N, O (left panel) and Ga, Ge and Se (right panel) doped arsenene.	63
3.4	The adsorption energy of hydrogen and oxygen on pristine and B, N, O, Ga, Ge and Se doped arsenene.	64
3.5	(a) shows the density of states of isolated H and H adsorbed on pristine arsenene and doped arsenene and (b) the density of states of isolated O and O adsorbed on pristine and doped arsenene.	67

3.6	The optimized geometries of pristine (a) ZrS <sub>2</sub> , (b) ZrSSe and (C) ZrSe <sub>2</sub> . Box in the top represents the unit cell considered for the calculations	68
3.7	The calculated band gap of pristine (a) ZrS <sub>2</sub> , (b) ZrSSe and (C) ZrSe <sub>2</sub> . Red and blue curves represent conduction and valence bands respectively.	70
3.8	The calculated PDOS of hydrogen adsorbed at basal plane and edge-site of (a) ZrS <sub>2</sub> , (b) ZrSSe and (C) ZrSe <sub>2</sub> .	73
3.9	Top and side views of the optimized geometries of doped (a) ZrS <sub>2</sub> , (b) ZrSSe and (C) ZrSe <sub>2</sub> ; purple sphere represents dopants (Nb, Pt and W), sky blue sphere represents S atoms, white atoms represent Se and Green sphere represents Zr atoms respectively. Box in the top represents the unit cell considered for the calculations.	75
3.10	The calculated PDOS of functionalized (a) ZrS <sub>2</sub> , (b) ZrSSe and (C) ZrSe <sub>2</sub> with dopant Nb, Pt and W respectively.	77
4.1	Top and side view of optimized structure of monolayer buckled hexagonal (hb) (a) bismuthine (b) bismuth arsenide and bismuth antimonide. Purple, red and green balls represent bismuth, arsenic and antimony atoms respectively.	89
4.2	Electronic band structure of 2D monolayer (a) Bi, (b) BiAs and (c) BiSb.	90
4.3	(a) real part of dielectric constant, (b) imaginary part of dielectric constant and (c) absorption coefficient of monolayer Bi, BiAs and BiSb.	91
4.4	The calculated VBM, CB at $\Gamma$ , CB at valley and CB at $K$ as a function of strain for (a) Bi, (b) BiAs and (c) BiSb	93
4.5	The electronic band structure of (a) Bi, (b) BiAs and (c) BiSb under compressive strain where they turn into indirect band gap semiconductor	94
4.6	Phonon dispersion curve as a function of strain for Bi, BiAs and BiSb.	95
4.7	The calculated elastic constants as a function of strain for (a) Bi, (b) BiAs and (c) BiSb.	98
4.8	The calculated (a) Poisson's ratio (b) Young's modulus (c) Bulk modulus and (d) Shear modulus as a function of strain for Bi, BiAs and BiSb respectively.	99

5.1	The optimized structure of hetero-structure Si/SnSe <sub>2</sub> , (a) side view and (b) top view.	110
5.2	The electronic band structure of (a) silicene, (b) SnSe <sub>2</sub> and hetero-structure Si/SnSe <sub>2</sub> ; red (blue) and brown (violet) represents conduction bands (valance bands) of Silicene and SnSe <sub>2</sub> respectively.	111
5.3	(a) Total density of states of SnSe <sub>2</sub> , silicene and hetero-structure Si/SnSe <sub>2</sub> and (b) partial density of states of hetero-structure Si/SnSe <sub>2</sub>	113
5.4	Top and side view of (a) initial and (b) optimized structure of Cl-intercalated hetero-structure Si/SnSe <sub>2</sub> respectively.	115
5.5	(a) The electronic bands structure and (b) partial density of state (PDOS) of Cl-intercalated hetero-structure Si/SnSe <sub>2</sub> respectively.	117
5.6	The charge density plot of Cl-intercalated hetero-structure Si/SnSe <sub>2</sub> .	118
5.7	Top and side view of optimized structure of P-intercalated hetero-structure Si/SnSe <sub>2</sub> .	119
5.8	(a) The electronic bands structure and (b) partial density of state (PDOS) of Cl-intercalated hetero-structure Si/SnSe <sub>2</sub> respectively.	120
5.9	The charge density plot of P-intercalated hetero-structure Si/SnSe <sub>2</sub> .	121
5.10	Top and side view of optimized structure of NH <sub>3</sub> <sup>a</sup> -intercalated hetero-structure Si/SnSe <sub>2</sub> .	122
5.11	The charge density plot of NH <sub>3</sub> <sup>a</sup> -intercalated hetero-structure Si/SnSe <sub>2</sub> .	123
5.12	(a) The electronic bands structure and (b) partial density of state (PDOS) of NH <sub>3</sub> <sup>a</sup> -intercalated hetero-structure Si/SnSe <sub>2</sub> respectively.	124
5.13	Top and side view of optimized structure of NH <sub>3</sub> <sup>b</sup> -intercalated hetero-structure Si/SnSe <sub>2</sub> .	125
5.14	The charge density plot of P-intercalated hetero-structure Si/SnSe <sub>2</sub> .	126
5.15	(a) The electronic bands structure and (b) partial density of state (PDOS) of NH <sub>3</sub> <sup>b</sup> -intercalated hetero-structure Si/SnSe <sub>2</sub> respectively.	127
5.16	Top and side view of optimized structure of CO adsorbed over Si/SnSe <sub>2</sub> .	128

5.17	The partial density of state (PDOS) of Co adsorbed over Silicene.	129
5.18	Top and side view of optimized structure of Co adsorbed over (a) SnSe <sub>2</sub> , (b) Si/SnSe <sub>2</sub> (c) Si/Cl/SnSe <sub>2</sub> (d) Si/P/SnSe <sub>2</sub> (e) Si/NH <sub>3</sub> <sup>a</sup> /SnSe <sub>2</sub> and (f) Si/NH <sub>3</sub> <sup>b</sup> /SnSe <sub>2</sub> respectively.	131
5.19	The partial density of state (PDOS) of Co adsorbed over (a) SnSe <sub>2</sub> , (b) Si/SnSe <sub>2</sub> (c) Si/Cl/SnSe <sub>2</sub> (d) Si/P/SnSe <sub>2</sub> (e) Si/NH <sub>3</sub> <sup>a</sup> /SnSe <sub>2</sub> and (f) Si/NH <sub>3</sub> <sup>b</sup> /SnSe <sub>2</sub> respectively.	132
6.1	Crystal structure of (a) CsPbI <sub>3</sub> and (b) CH <sub>3</sub> NH <sub>3</sub> PbI <sub>3</sub> .	140
6.2	Crystal structure of MAPI (a) cubic, (b) tetragonal, (c) orthorhombic and (d) hexagonal	141
6.3	Atomic model for the cubic phase of MAPI. (a) bulk, (b) two-dimensional and (c) one-dimensional	145
6.4	Electronic band structure of cubic MAPI. (a) bulk, (b) two-dimensional and (c) one-dimensional MAPI.	147
6.5	Partial electronic density of states (PDOS) for bulk, two-dimensional and one-dimensional MAPI.	148
6.6	(a) Calculated real part of di-electric constant and (b) imaginary part of di-electric constant of bulk, 2D and 1D MAPI	150
6.7	(a) Absorption coefficient and (b) joint density of state (JDOS) of bulk, 2D and 1D MAPI	151
6.8	(a) Change in bandgap as function of strain, (b) The calculated energies for VBM, CBM at <b>X</b> and CBM at <b>Γ</b> for MAPI 1D as function of uniaxial strain and (c) The calculated energies for VBM, CBM at <b>M</b> and CBM at valley for MAPI 2D as function of biaxial strain.	154
6.9	(a) Conduction and valence bands of MAPI 1D under different uniaxial strain and (b) Conduction and the valence bands of MAPI 2D under biaxial strain.	155
6.10	Layered electronic band structures of (a) monolayer, (b) bilayer and (c) trilayer of 2D MAPI.	157
7.1	Adsorption energy of hydrogen and oxygen on pristine and B, N, O, Ga, Ge and Se doped arsenene.	165