

List of Figures

Figures	Title	page
1.1	(a) Top view, (b) side view and (c) band structure along high symmetry points of BZ of graphene.	2
1.2	Schematic representations of few selected 2D monolayers and corresponding electronic band gap	3
2.1	Periodic table representing the possible transition metals and chalcogen atoms, top view of hexagonal and trigonal phase and corresponding possible symmetry	6
2.2	Band gap variation of monolayer, bilayer, trilayer and quad layer of WS ₂ without and with SOC.	8
2.3	Schematic representation of (a) light absorption and photoluminescence, and (b) Raman scattering.	9
2.4	Band gap variation against the uniaxial and biaxial strain of MX ₂ (M = Mo, W; X = S, Se and Te) monolayers	10
2.5	Point defects and antisite defects observed in MoS ₂ monolayer using the STM analysis	10
2.6	Schematic representation of applications of TMDs based monolayers	11
2.7	(a) Steps used for synthesis process, (b) Raman spectrum, (c) Photoluminescence spectrum and (d) Angular dark field STEM of MoS ₂ monolayer	12
2.8	Theoretically explored applications of JTMDs monolayers.	13
3.1	Density functional theory based per year publications from 2000 to 2019 (Source: Web of Science)	15
3.2	Schematic representation of Schrödinger system for electrons and nuclei interaction	16
3.3	Jacob's ladder of exchange correlation functional	19
3.4	Flow chart of self-consistent field cycle iteration	20
3.5	Schematic representation of approximation of full potential to pseudopotentials	21
3.6	Flow chart diagram of Density Functional Perturbation Theory	23
4.1	Optimized geometries and corresponding structural parameters of (a) WS ₂ , (b) WSSe and (c) WSe ₂ monolayer; (d) Schematic representation of hexagonal BZ.	27
4.2	Schematic representation of vibrational modes of WS ₂ monolayer	27
4.3	Phonon band dispersion of (a) WS ₂ , (b) WSSe, and (c) WSe ₂ monolayer	28
4.4	(a), (c) and (e) are the band structure and (b), (d) and (f) are the PDOS of WS ₂ , WSSe and WSe ₂ monolayers, respectively.	28
4.5	Band structure of (a) WS ₂ , (b) WSSe, and (c) WSe ₂ monolayers using GGA+SOC	29
4.6	Phonon band dispersion (a) 6% compressive strain (b) 2% compressive strain (c) 2% tensile strain and (d) 6% tensile strain for WSSe monolayer	29
4.7	Electronic band structure of (a) and (b) at 1.5% compression strain and 0.5% tensile strain, WS ₂ monolayer, respectively; (c) and (d) 1% compression strain and 1% tensile strain, WSSe monolayer, respectively; (e) and (f) at 1.5% compression strain at 2.5% tensile strain, WSe ₂ monolayer, respectively.	30
4.8	(a) Band gap, (b) effective mass and (c) mobility variation of WS ₂ , WSSe and WSe ₂ monolayers.	31
5.1	Schematic representation of initial geometry of H ₂ S, NH ₃ , NO ₂ and NO molecules	34
5.2	(a) and (b) are the band structure; (c) and (d) are PDOS of WSSe@Ses and WSSe@Sse monolayer, respectively.	35
5.3	Optimized structures of H ₂ S (a–d), NH ₃ (e–h), NO ₂ (i–l) and NO (m–p) molecules adsorbed on the selenium and sulfur surfaces of the WSSe monolayer.	36
5.4	(a–d) H ₂ S, (e–h) NH ₃ , (i–l) NO ₂ and (m–p) NO charge density difference.	37
5.5	Comparison of SPDOS of pristine monolayer and molecule adsorbed monolayers (a&b) H ₂ S, (c&d) NH ₃ , (e&f) NO ₂ and (g–h) NO	38
5.6	(a) Adsorption energy and (b–d) temperature dependent recovery times of molecules adsorb on selenium and sulfur surface of monolayer.	38
5.7	(a–d) Optimized geometries, (e–h) charge density difference and (i–l) SPDOS of gas molecules adsorb on WSSe@Ses monolayer.	40

5.8	(a-d) Optimized geometries, (e-h) charge density difference and (i-l) SPDOS of gas molecules adsorb on WSSe@Sse monolayer.	41
5.9	(a) and (b) are the band structure; (c) and (d) are PDOS of MoSSe@Sev and MoSSe@(S/Se)v monolayer, respectively.	42
5.10	Optimized geometries and charge density difference of H ₂ S adsorb on MoSSe (a&b), NH ₃ adsorb on MoSSe (c&d), NO ₂ adsorb on MoSSe (e&f) and NO adsorb on MoSSe (g&h).	43
5.11	Comparison of band structure of pristine monolayer with the gas molecule adsorbs on MoSSe monolayer (a) H ₂ S, (b) NH ₃ , (c) NO ₂ and NO.	44
5.12	(a) Adsorption energy and (b) vertical height of gas molecules adsorb on pristine MoSSe monolayer	45
5.13	Optimized geometries and charge density difference of H ₂ S (a&b), NH ₃ (c&d), NO ₂ (e&f) and NO (g&h) adsorb on MoSSe@Vse monolayer.	46
5.14	Optimized geometries and charge density difference of H ₂ S (a&b), NH ₃ (c&d), NO ₂ (e&f) and NO (g&h) adsorb on MoSSe@V _(S/Se) monolayer.	47
5.15	Comparison of band structure of pristine monolayer with the gas molecule adsorbs on MoSSe@V _{se} monolayer (a) H ₂ S, (b) NH ₃ , (c) NO ₂ and (d) NO.	47
5.16	Comparison of band structure of pristine monolayer with the gas molecule adsorb on MoSSe@V _(S/Se) monolayer (a) H ₂ S, (b) NH ₃ , (c) NO ₂ and (d) NO.	48
5.17	(a) Adsorption energy and (b) vertical height of gas molecules adsorb on MoSSe@V _{se} and MoSSe@V _(S/Se) monolayer.	48
6.1	Schematic diagram and corresponding structural parameters of (a) bulk WS ₂ and (b) bulk WSe ₂ .	52
6.2	(a) Band structure of WS ₂ (b) TDOS & PDOS of bulk WS ₂ (c) Band structure of WSe ₂ and (b) TDOS & PDOS of bulk WSe ₂	53
6.3	(a) Band structure of WSSe (b) TDOS & PDOS of WSSe monolayer, (c) band structure of WSeTe and (b) TDOS & PDOS of WSeTe monolayer.	54
6.4	Absorption spectra of bulk WS ₂ , (b) absorption spectra of bulk WSe ₂ and (c) absorption spectra of WSSe and WSeTe monolayers.	55
6.5	(a) Schematic representation of solar cell device, (b) band alignment at interface (c) J-V curve and (d) EQE of TCO/WSSe/WS ₂ , TCO/WSeTe/WS ₂ , TCO/WSSe/WSe ₂ and TCO/WSeTe/WSe ₂ solar cell devices.	57
6.6	Effect of acceptor layer thickness on (a) efficiency (b) open circuit voltage and (c) short circuit current of TCO/WSSe/WS ₂ , TCO/WSeTe/WS ₂ , TCO/WSSe/WSe ₂ and TCO/WSeTe/WSe ₂ solar cell devices.	58
6.7	Effect of acceptor layer carrier concentration on (a) efficiency (b) open circuit voltage and (c) short circuit current of TCO/WSSe/WS ₂ , TCO/WSeTe/WS ₂ , TCO/WSSe/WSe ₂ and TCO/WSeTe/WSe ₂ solar cell devices.	58
6.8	Contour plot of interface recombination speed at interface versus minority carrier life time of (a) AZO/WSSe/WS ₂ (b) AZO/WSeTe/WS ₂ (c) AZO/WSSe/WSe ₂ and (d) AZO/WSeTe/WSe ₂ solar cell devices.	59
6.9	Contour plot of an acceptor layer carrier concentration versus thickness of buffer layer of (a) AZO/WSSe/WS ₂ (b) AZO/WSeTe/WS ₂ (c) AZO/WSSe/WSe ₂ and (d) AZO/WSeTe/WSe ₂ solar cell devices.	60
6.10	(a) J-V and (b) QE plot based on the optimized parameters of considered solar cells.	61
7.1	Phonon band dispersion curve of Janus WSSe monolayer.	64
7.2	(a) Carrier concentration, (b) density of states, (c) Seebeck coefficient, (d) electrical conductivity, (e) electronic thermal conductivity, (f) lattice thermal conductivity, (g) power factor and (h) figure of merit versus chemical potential of unstrained WSSe monolayer.	65
7.3	Cumulative thermal conductivity versus mean free path of WSSe monolayer at (a) 300K and (b) 1500K.	66
7.4	Comparison of phonon band softening and/or hardening under the compressive and tensile strains. Here K refers Γ -M-K- Γ direction.	68
7.5	Variation of the valence and conduction band edges under the biaxial compressive and tensile strains	68
7.6	Strain dependent Seebeck coefficients for (a) p-type carriers, (b) n-type carriers and (c) band gap and Seebeck coefficient.	69
7.7	Chemical potentials dependent electrical conductivity of WSSe monolayer at different temperatures for (a) - 6%, (b) - 4%, (c) -2%, (d) 2%, (e) 4% and (f) 6% strain.	70

7.8	Chemical potentials dependent electronic thermal conductivity of WSSe monolayer at different temperatures for (a) – 6%, (b) - 4%, (c) -2%, (d) 2%, (e) 4% and (f) 6% strain.	71
7.9	The variation in (a) frequency of LA, TA and ZA modes and group velocity against strain and (b) Lattice thermal conductivity against temperature at different strain values for WSSe monolayer.	72
7.10	Chemical potentials dependent power factor of WSSe monolayer at different temperatures for (a) – 6%, (b) - 4%, (c) -2%, (d) 2%, (e) 4% and (f) 6% strain.	73
7.11	Chemical potentials dependent figure of merit of WSSe monolayer at different temperatures for (a) – 6%, (b) - 4%, (c) -2%, (d) 2%, (e) 4% and (f) 6% strain.	74
7.12	(a) Schematic representation of WSSe monolayer based thermoelectric device, and (b) the comparison of thermoelectric device efficiency against temperature for unstrained and strained WSSe monolayers.	74
8.1	Explored applications of Janus monolayers	78
8.2	The potential future possibilities with Janus monolayers	79