

WSe <sub>2</sub>		
Property	Description/Value	
	Bulk	Monolayer
Lattice constant (a)	3.28 Å [1]	3.32 Å [2]
Molar mass	341.76 g/mol [3, 4]	341.76 g/mol [3, 4]
Band gap type	Indirect [5]	Direct [5]
Band gap energy	1.2 eV (experimental) [6]	1.65 eV (experimental) [5] 1.25 eV (calculation) [2]
Coordination geometry	Trigonal prismatic (W <sup>IV</sup> ), Pyramidal (Se <sup>-2</sup> ) [3, 4, 7]	Trigonal prismatic (W <sup>IV</sup> ), Pyramidal (Se <sup>-2</sup> ) [3, 4, 7]
Crystal structure	hP6, space group P6 <sub>3</sub> /mmc, No 194 [3,7]	hP6, space group P6 <sub>3</sub> /mmc, No 194 [3, 7]
Appearance	Grey to black solid [3, 7]	-----
Group	Transition Metal Dichalcogenide [7]	Transition Metal Dichalcogenide [7]
Spin-orbit splitting	-----	0.47 eV [2]
Poisson's ratio	-----	0.19 [2]
Cohesive energy per unit cell	-----	15.45 eV [2]
Charge transfer of W atom	0.96 e [2]	0.96 e [2]
In-plane stiffness	-----	115.52 N/m [2]
Density	9.32 g/cm <sup>3</sup> [3]	9.32 g/cm <sup>3</sup> [3]
Melting point	1500 °C [8]	-----
Exciton binding energy	-----	0.79 eV [9]
W-Se bond length	-----	2.55 Å [2]
Dielectric constant ( $\epsilon$ )	-----	Real part ( $\epsilon_1$ )=~22, Imaginary part ( $\epsilon_2$ )=~10 (at 1.7 eV incident photon energy) [10]
Effective masses	-----	$m_e = 0.53 m_o$ , $m_h = 0.52 m_o$ [11]
Effective Bohr radius	-----	-----
Thermal expansion coefficient	-----	$11.08 \times 10^{-6} /^\circ\text{C}$ [12]
Bulk Modulus (B)	-----	-----
Refractive Index	-----	5.68 [13]
Carrier mobility in WSe <sub>2</sub>		
Thicknesses	BN/SiO <sub>2</sub> /Si substrate	SiO <sub>2</sub> /Si Substrate
8 nm	-----	~350 cm <sup>2</sup> /V.Sec (hole) [14]
Monolayer	~31 cm <sup>2</sup> /V.Sec [15]	-----
Bulk	-----	-----

## References:

- [1] R. Coehoorn, C. Haas, J. Dijkstra, and C. J. F. Flipse, R. A. de Groot, A. Wold "Electronic structure of MoSe<sub>2</sub>, MoS<sub>2</sub>, and WSe<sub>2</sub>. I. Band-structure calculations and photoelectron spectroscopy" PHYSICAL REVIEW B, 35, 12, 6195-6202, 1987. DOI:<http://dx.doi.org/10.1103/PhysRevB.35.6195>
- [2] Jun Kang, Sefaattin Tongay, Jian Zhou, Jingbo Li, and Junqiao Wu, "Band offsets and heterostructures of two-dimensional semiconductors" APPLIED PHYSICS LETTERS 102, 012111 2013. DOI: <http://dx.doi.org/10.1063/1.4774090>
- [3] Schutte, W.J.; De Boer, J.L.; Jellinek, F. "Crystal Structures of Tungsten Disulfide and Diselenide". *Journal of Solid State Chemistry*, 70: 207–209, 1986. doi:10.1016/0022-4596(87)90057-0
- [4] N. N. Greenwood; A. Earnshaw "Chemistry of the Elements" Elsevier, 1997. ISBN 978-0-08-050109-3.
- [5] Weijie Zhao, Zohreh Ghorannevis, Leiqiang Chu, Minglin Toh, Christian Kloc, Ping-Heng Tan, and Goki Eda "Evolution of Electronic Structure in Atomically Thin Sheets of WS<sub>2</sub> and WSe<sub>2</sub>" ACS Nano VOL. 7, NO. 1, 791–797, 2013. DOI: 10.1021/nn305275h
- [6] Hui Fang, Steven Chuang, Ting Chia Chang, Kuniharu Takei, Toshitake Takahashi, and Ali Javey "High-Performance Single Layered WSe<sub>2</sub> p-FETs with Chemically Doped Contacts" Nano Lett. 12, 3788–3792, 2012. DOI: [dx.doi.org/10.1021/nl301702r](http://dx.doi.org/10.1021/nl301702r)
- [7] Wang, Q. H; Kalantar-Zadeh; Kis, A; Coleman, J.N.; Strano, M.S. "Electronics and Optoelectronics of Two-dimensional Transition Metal Dichalcogenides" Nature Nanotechnology, 7, 699-712, 2007. doi:10.1038/nnano.2012.193
- [8] S. Kumar and U. Schwingenschlo," Thermoelectric Response of Bulk and Monolayer MoSe<sub>2</sub> and WSe<sub>2</sub>" Chem. Mater. 27, 1278–1284, 2015. DOI: 10.1021/cm504244b
- [9] A.T. Hanbicki, M. Currie, G. Kioseoglou, A. L .Friedman, B.T. Jonker "Measurement of high exciton binding energy in the monolayer transition-metal dichalcogenides WS<sub>2</sub> and WSe<sub>2</sub>" Solid State Communications 203, 16–20, 2015. DOI: <http://dx.doi.org/10.1016/j.ssc.2014.11.005>
- [10] Yilei Li, Alexey Chernikov, Xian Zhang, Albert Rigosi, Heather M. Hill, Arend M. van der Zande, Daniel A. Chenet, En-Min Shih, James Hone, and Tony F. Heinz, Measurement of the optical dielectric function of monolayer transition-metal dichalcogenides: MoS<sub>2</sub>, MoSe<sub>2</sub>, WS<sub>2</sub>, and WSe<sub>2</sub>" PHYSICAL REVIEW B 90, 205422 (2014). DOI: 10.1103/PhysRevB.90.205422
- [11] Ashwin Ramasubramaniam "Large excitonic effects in monolayers of molybdenum and tungsten dichalcogenides" PHYSICAL REVIEW B 86, 115409 2012. DOI: 10.1103/PhysRevB.86.115409
- [12] S. H. EL-MAHALAWY AND B. L. EVANS "The Thermal Expansion of 2H-MoS<sub>2</sub>, 2H-MoSe<sub>2</sub> and 2H-WSe<sub>2</sub> between 20 and 800°C" J. Appl. Cryst. 9, 403, 1976.

- [13] Hsiang-Lin Liu, Chih-Chiang Shen, Sheng-Han Su, Chang-Lung Hsu, Ming-Yang Li, and Lain-Jong Li, “Optical properties of monolayer transition metal dichalcogenides probed by spectroscopic ellipsometry” APPLIED PHYSICS LETTERS 105, 201905, 2014. DOI: 10.1063/1.4901836
- [14] N. R. Pradhan, D. Rhodes, S. Memaran, J. M. Poumirol, D. Smirnov, S. Talapatra, S. Feng, N. Perea-Lopez, A. L. Elias, M. Terrones, P. M. Ajayan & L. Balicas “Hall and field-effect mobilities in few layered p-WSe<sub>2</sub> field-effect transistors” SCIENTIFIC REPORTS, 5, 8979, 2015. DOI:10.1038/srep08979
- [15] Bilu Liu, Yuqiang Ma, Anyi Zhang, Liang Chen, Ahmad N. Abbas, Yihang Liu, Chenfei Shen, Haochuan Wan, and Chongwu Zhou “High-Performance WSe<sub>2</sub> Field-Effect Transistors via Controlled Formation of In-Plane Heterojunctions” ACS Nano 10, 5153–5160, 2016. DOI: 10.1021/acsnano.6b00527