References

Aierken, Y., Çakir, D., & Peeters, F. M. (2016). Strain enhancement of acoustic phonon limited mobility in monolayer TiS3. *Physical Chemistry Chemical Physics*, *18*(21), 14434–14441. https://doi.org/10.1039/c6cp01809b

Aivazian, G., Gong, Z., Jones, A. M., Chu, R. L., Yan, J., Mandrus, D. G., … Xu, X. (2015). Magnetic control of valley pseudospin in monolayer WSe 2. *Nature Physics*, *11*(2), 148–152. https://doi.org/10.1038/nphys3201

Akama, T., Okita, W., Nagai, R., Li, C., Kaneko, T., & Kato, T. (2017). Schottky solar cell using few-layered transition metal dichalcogenides toward large-scale fabrication of semitransparent and flexible power generator. *Scientific Reports*, *7*(1), 1–10. https://doi.org/10.1038/s41598-017-12287-6

Allain, A., & Kis, A. (2014). Electron and hole mobilities in single-layer WSe2. *ACS Nano*, *8*(7), 7180–7185. https://doi.org/10.1021/nn5021538

Alsaleh, N. M., Shoko, E., & Schwingenschlögl, U. (2019). Pressure-induced conduction band convergence in the thermoelectric ternary chalcogenide CuBiS2. *Physical Chemistry Chemical Physics*, *21*(2), 662–673. https://doi.org/10.1039/c8cp05818k

Amin, B., Kaloni, T. P., & Schwingenschlögl, U. (2014). Strain engineering of WS2, WSe2, and WTe2. *RSC Advances*, *4*(65), 34561–34565. https://doi.org/10.1039/c4ra06378c

Babar, V., Vovusha, H., & Schwingenschlögl, U. (2019). Density Functional Theory Analysis of Gas Adsorption on Monolayer and Few Layer Transition Metal Dichalcogenides: Implications for Sensing. *ACS Applied Nano Materials*, *2*(9), 6076–6080. https://doi.org/10.1021/acsanm.9b01642

Balendhran, S., Walia, S., Nili, H., Sriram, S., & Bhaskaran, M. (2015). Elemental analogues of graphene: Silicene, germanene, stanene, and phosphorene. *Small*, *11*(6), 640–652. https://doi.org/10.1002/smll.201402041

Baroni, S., De Gironcoli, S., Dal Corso, A., & Giannozzi, P. (2001). Phonons and related crystal properties from density-functional perturbation theory. *Reviews of Modern Physics*, *73*(2), 515–562. https://doi.org/10.1103/RevModPhys.73.515

Basharnavaz, H., Habibi-Yangjeh, A., & Mousavi, M. (2018). Ni, Pd, and Pt-embedded graphitic carbon nitrides as excellent adsorbents for HCN removal: A DFT study. *Applied Surface Science*, *456*(June), 882–889. https://doi.org/10.1016/j.apsusc.2018.06.159

Bera, J., & Sahu, S. (2019). Strain induced valley degeneracy: A route to the enhancement of thermoelectric properties of monolayer WS2. *RSC Advances*, *9*(43), 25216–25224. https://doi.org/10.1039/c9ra04470a

Bernardi, M., Palummo, M., & Grossman, J. C. (2013). Extraordinary sunlight absorption and one nanometer thick photovoltaics using two-dimensional monolayer materials. *Nano Letters*, *13*(8), 3664–3670. https://doi.org/10.1021/nl401544y

Bertolazzi, S., Brivio, J., & Kis, A. (2011). Stretching and breaking of ultrathin MoS 2. *ACS Nano*, *5*(12), 9703–9709. https://doi.org/10.1021/nn203879f

Bhattacharyya, S., Pandey, T., & Singh, A. K. (2014). Effect of strain on electronic and thermoelectric properties of few layers to bulk MoS2. *Nanotechnology*, *25*(46). https://doi.org/10.1088/0957-4484/25/46/465701

Bianco, E., Butler, S., Jiang, S., Restrepo, O. D., Windl, W., & Goldberger, J. E. (2013). Stability and exfoliation of germanane: A germanium graphane analogue. *ACS Nano*, *7*(5), 4414–4421. https://doi.org/10.1021/nn4009406

Bilc, D. I., Mahanti, S. D., & Kanatzidis, M. G. (2006). Electronic transport properties of PbTe and AgPbm SbTe 2+m systems. *Physical Review B - Condensed Matter and Materials Physics*, *74*(12). https://doi.org/10.1103/PhysRevB.74.125202

Blaha, P., & Madsen, G. (2016). *WIEN2k* (Vol. 1).

Bosi, M. (2015). Growth and synthesis of mono and few-layers transition metal dichalcogenides by vapour techniques: A review. *RSC Advances*, *5*(92), 75500–75518. https://doi.org/10.1039/c5ra09356b

Bruzzone, S., & Fiori, G. (2011). Ab-initio simulations of deformation potentials and electron mobility in chemically modified graphene and two-dimensional hexagonal boron-nitride. *Applied Physics Letters*, *99*(22), 16–19. https://doi.org/10.1063/1.3665183

Burgelman, M., Decock, K., Niemegeers, A., Verschraegen, J., & Degrave, S. (2018). *SCAPS manual*. (january).

Caillat, T., Borshchevsky, A., & Fleurial, J. P. (1996). Properties of single crystalline semiconducting CoSb3. *Journal of Applied Physics*, *80*(8), 4442–4449. https://doi.org/10.1063/1.363405

Camilli, L., & Passacantando, M. (2018). Advances on sensors based on carbon nanotubes. *Chemosensors*, *6*(4), 1–17. https://doi.org/10.3390/chemosensors6040062

Cao, Q., Dai, Y. W., Xu, J., Chen, L., Zhu, H., Sun, Q. Q., & Zhang, D. W. (2017). Realizing Stable p-Type Transporting in Two-Dimensional WS2Films. *ACS Applied Materials and Interfaces*, *9*(21), 18215–18221.

https://doi.org/10.1021/acsami.7b03177
Cappelluti, E., Roldán, R., Silva-Guillén, J. A., Ordejón, P., & Guinea, F. (2013). Tight-binding model and direct-gap/indirect-gap transition in single-layer and multilayer MoS2. *Physical Review B - Condensed Matter and Materials Physics*, *88*(7), 1–18. https://doi.org/10.1103/PhysRevB.88.075409
Carozo, V., Wang, Y., Fujisawa, K., Carvalho, B. R., McCreary, A., Feng, S., … Terrones, M. (2017). Optical identification of sulfur vacancies: Bound excitons at the edges of monolayer tungsten disulfide. *Science Advances*, *3*(4), 1–10. https://doi.org/10.1126/sciadv.1602813
Castro Neto, A. H., Guinea, F., Peres, N. M. R., Novoselov, K. S., & Geim, A. K. (2009). The electronic properties of graphene. *Reviews of Modern Physics*, *81*(1), 109–162. https://doi.org/10.1103/RevModPhys.81.109
Chang, C., & Fan, X. (2013). Orbital analysis of electronic structure and phonon dispersion in MoS 2 , MoSe 2 , WS 2 , and WSe 2 monolayers under strain. *Physical Review B*, *195420*, 1–9. https://doi.org/10.1103/PhysRevB.88.195420
Chaput, L., Pécheur, P., Tobola, J., & Scherrer, H. (2005). Transport in doped skutterudites: Ab initio electronic structure calculations. *Physical Review B - Condensed Matter and Materials Physics*, *72*(8). https://doi.org/10.1103/PhysRevB.72.085126
Chaurasiya, R., & Dixit, A. (2019). Defect engineered MoSSe Janus monolayer as a promising two dimensional material for NO2 and NO gas sensing. *Applied Surface Science*, *490*(May), 204–219. https://doi.org/10.1016/j.apsusc.2019.06.049
Chaurasiya, R., & Dixit, A. (2020). Ultrahigh sensitivity with excellent recovery time for NH 3 and NO 2 in pristine and defect mediated Janus WSSe monolayer . *Physical Chemistry Chemical Physics*, (2), 13903–13922. https://doi.org/10.1039/d0cp02063j
Chaurasiya, R., Dixit, A., & Pandey, R. (2018a). Strain-mediated stability and electronic properties of WS 2 , Janus WSSe and WSe 2 monolayers. *Superlattices and Microstructures*, *122*(May), 268–279. https://doi.org/10.1016/j.spmi.2018.07.039
Chaurasiya, R., Dixit, A., & Pandey, R. (2018b). Strain-mediated stability and electronic properties of WS2, Janus WSSe and WSe2 monolayers. *Superlattices and Microstructures*, *122*(May), 268–279. https://doi.org/10.1016/j.spmi.2018.07.039
Cheng, Y. C., Zhu, Z. Y., Tahir, M., & Schwingenschlögl, U. (2013). Spin-orbit-induced spin splittings in polar transition metal dichalcogenide monolayers. *Epl*, *102*(5). https://doi.org/10.1209/0295-5075/102/57001
Cho, B., Hahm, M. G., Choi, M., Yoon, J., Kim, A. R., Lee, Y. J., … Kim, D. H. (2015). Charge-transfer-based gas sensing using atomic-layer MoS2. *Scientific Reports*, *5*(2), 8052. https://doi.org/10.1038/srep08052
Coehoorn, R., Haas, C., Dijkstra, J., Flipse, C. J. F., De Groot, R. A., & Wold, A. (1987). Electronic structure of MoSe2, MoS2, and WSe2. I. Band-structure calculations and photoelectron spectroscopy. *Physical Review B*, *35*(12), 6195–6202. https://doi.org/10.1103/PhysRevB.35.6195
Coleman, J. N., Lotya, M., O'neill, A., Bergin, S. D., King, P. J., Khan, U., … Nicolosi, V. (2011). Two-Dimensional Nanosheets Produced by Liquid Exfoliation of Layered Materials. *Science*, *331*(February), 568–571.
Courel, M., Andrade-Arvizu, J. A., & Vigil-Galán, O. (2015). Loss mechanisms influence on Cu2ZnSnS4/CdS-based thin film solar cell performance. *Solid-State Electronics*, *111*, 243–250. https://doi.org/10.1016/j.sse.2015.05.038
Cozza, D., Ruiz, C. M., Duch, D., Simon, J. J., & Escoubas, L. (2016). Modeling the Back Contact of Cu 2 ZnSnSe 4 Solar Cells. *IEEE Journal of Photovoltaics*, *2576678*(1), 1–6. https://doi.org/10.1109/JPHOTOV.2016.2576678
Cui, X., Zeng, H., Dai, J., Yao, W., He, R., Liu, G.-B., … Xie, L. (2013). Optical signature of symmetry variations and spin-valley coupling in atomically thin tungsten dichalcogenides. *Scientific Reports*, *3*(1), 2–6. https://doi.org/10.1038/srep01608
D. T. Morelli, T. Caillat, J.-P. Fleurial, A. Borshchevsky, and J. Vandersande, B. C. and C. U. (1995). Low-temperature transport propertIes ofp-type CoSb3. *PHYSICAL REVIEW B*, *51*(15), 9622–9628.
Das, V. D., & Soundararajan, N. (1987). Size and temperature effects on the Seebeck coefficient of thin bismuth films. *Physical Review B*, *35*(12), 5990–5996. https://doi.org/10.1103/PhysRevB.35.5990
Devadasan, J. J., Sanjeeviraja, C., & Jayachandran, M. (2001). Electrodeposition of p-WS2 thin film and characterisation. *Journal of Crystal Growth*, *226*(1), 67–72. https://doi.org/10.1016/S0022-0248(01)00851-X
Dimple, Jena, N., & De Sarkar, A. (2017). Compressive strain induced enhancement in thermoelectric-power-factor in monolayer MoS2 nanosheet. *Journal of Physics Condensed Matter*, *29*(22). https://doi.org/10.1088/1361-648X/aa6cbc
Dong, L., Lou, J., & Shenoy, V. B. (2017). Large In-Plane and Vertical Piezoelectricity in Janus Transition Metal Dichalchogenides. *ACS Nano*, *11*(8), 8242–8248. https://doi.org/10.1021/acsnano.7b03313
Dove, M. T. (1393). Introduction to the theory of lattice dynamics. In *Cambridge University Press* (Vol. 4). https://doi.org/10.1051/sfn/201112007
Er, D., Ye, H., Frey, N. C., Kumar, H., Lou, J., & Shenoy, V. B. (2018). Prediction of Enhanced Catalytic Activity for Hydrogen Evolution Reaction in Janus Transition Metal Dichalcogenides [Rapid-communication]. *Nano*

Letters, *18*, acs.nanolett.8b01335. https://doi.org/10.1021/acs.nanolett.8b01335
Fang, H., Chuang, S., Chang, T. C., Takei, K., Takahashi, T., & Javey, A. (2012). High-performance single layered WSe 2 p-FETs with chemically doped contacts. *Nano Letters*, *12*(7), 3788–3792. https://doi.org/10.1021/nl301702r
Feynman, R. P. (1939). Forces in molecules. *Physical Review*, *56*(4), 340–343. https://doi.org/10.1103/PhysRev.56.340
Furchi, M. M., Zechmeister, A. A., Hoeller, F., Wachter, S., Pospischil, A., & Mueller, T. (2017). Photovoltaics in Van der Waals Heterostructures. *IEEE Journal of Selected Topics in Quantum Electronics*, *23*(1). https://doi.org/10.1109/JSTQE.2016.2582318
Gan, Y., & Zhao, H. (2014). Chirality effect of mechanical and electronic properties of monolayer MoS2 with vacancies. *Physics Letters, Section A: General, Atomic and Solid State Physics*, *378*(38–39), 2910–2914. https://doi.org/10.1016/j.physleta.2014.08.008
Gandi, A. N., & Schwingenschlögl, U. (2014). WS2 as an excellent high-temperature thermoelectric material. *Chemistry of Materials*, *26*(22), 6628–6637. https://doi.org/10.1021/cm503487n
Gandi, A. N., & Schwingenschlögl, U. (2016). Electron dominated thermoelectric response in MNiSn (M: Ti, Zr, Hf) half-Heusler alloys. *Physical Chemistry Chemical Physics*, *18*(20), 14017–14022. https://doi.org/10.1039/c6cp01786j
Giannozzi, P., Baroni, S., Bonini, N., Calandra, M., Car, R., Cavazzoni, C., … Wentzcovitch, R. M. (2009a). QUANTUM ESPRESSO: A modular and open-source software project for quantum simulations of materials. *Journal of Physics Condensed Matter*, *21*(39). https://doi.org/10.1088/0953-8984/21/39/395502
Giannozzi, P., Baroni, S., Bonini, N., Calandra, M., Car, R., Cavazzoni, C., … Wentzcovitch, R. M. (2009b). QUANTUM ESPRESSO: A modular and open-source software project for quantum simulations of materials. *Journal of Physics Condensed Matter*, *21*(39), 395502. https://doi.org/10.1088/0953-8984/21/39/395502
Giannozzi, P., Baroni, S., Bonini, N., Calandra, M., Car, R., Cavazzoni, C., … Wentzcovitch, R. M. (2009c). QUANTUM ESPRESSO: A modular and open-source software project for quantum simulations of materials. *Journal of Physics Condensed Matter*, *21*(39). https://doi.org/10.1088/0953-8984/21/39/395502
Goldsmid, H. J., & Sharp, J. W. (1999). Estimation of the thermal band gap of a semiconductor from Seebeck measurements. *Journal of Electronic Materials*, *28*(7), 869–872. https://doi.org/10.1007/s11664-999-0211-y
Green, M. A. (1990). Intrinsic concentration, effective densities of states, and effective mass in silicon. *Journal of Applied Physics*, *67*(6), 2944–2954. https://doi.org/10.1063/1.345414
GRIMME, S. (2006). Semiempirical GGA-Type Density Functional Constructed with a Long-Range Dispersion Correction. *Journal of Computational Chemistry*, *27*(10), 1787–1799. https://doi.org/10.1002/jcc
Grund, D., & Erscheinungen, D. (1914). *d e r W&vneleitung in E r i s t n l l e n Von R. P e i e r l s*.
Guan, Z., Ni, S., & Hu, S. (2018). Tunable Electronic and Optical Properties of Monolayer and Multilayer Janus MoSSe as a Photocatalyst for Solar Water Splitting: A First-Principles Study. *Journal of Physical Chemistry C*, *122*(11), 6209–6216. https://doi.org/10.1021/acs.jpcc.8b00257
Guo, D., Hu, C., Xi, Y., & Zhang, K. (2013). Strain effects to optimize thermoelectric properties of doped Bi 2O2Se via tran-blaha modified Becke-Johnson density functional theory. *Journal of Physical Chemistry C*, *117*(41), 21597–21602. https://doi.org/10.1021/jp4080465
Guo, S.-D. (2018). *Biaxial strain tuned electronic structures and power factor in Janus Transition Metal Dichalchogenide monolayers*. Retrieved from http://arxiv.org/abs/1803.04147
Gupta, G. K., & Dixit, A. (2018). Theoretical studies of single and tandem Cu2ZnSn(S/Se)4junction solar cells for enhanced efficiency. *Optical Materials*, *82*(April), 11–20. https://doi.org/10.1016/j.optmat.2018.05.030
Gusakova, J., Wang, X., Shiau, L. L., Krivosheeva, A., Shaposhnikov, V., Borisenko, V., … Tay, B. K. (2017). Electronic Properties of Bulk and Monolayer TMDs: Theoretical Study Within DFT Framework (GVJ-2e Method). *Physica Status Solidi (A) Applications and Materials Science*, *214*(12), 1–7. https://doi.org/10.1002/pssa.201700218
He, X., Li, H., Zhu, Z., Dai, Z., Yang, Y., Yang, P., … Zhang, X. (2016). Strain engineering in monolayer WS2, MoS2, and the WS2/MoS2 heterostructure. *Applied Physics Letters*, *109*(17). https://doi.org/10.1063/1.4966218
Heikes, R. R., Ure, R. W., & Mullin, A. A. (1962). Thermoelectricity : Science and Engineering. *American Journal of Physics*, *30*, 78. https://doi.org/10.1119/1.1941916
Hellmann, H. (1933). Zur Rolle der kinetischen Elektronenenergie für die zwischenatomaren Kräfte. *Zeitschrift Für Physik*, *85*(3–4), 180–190. https://doi.org/10.1007/BF01342053
Henkelman, G., Arnaldsson, A., & Jónsson, H. (2006). A fast and robust algorithm for Bader decomposition of charge density. *Computational Materials Science*, *36*(3), 354–360. https://doi.org/10.1016/j.commatsci.2005.04.010
Hicks, L. D., Harman, T. C., & Dresselhaus, M. S. (1993). Use of quantum-well superlattices to obtain a high figure of merit from nonconventional thermoelectric materials. *Applied Physics Letters*, *63*(23), 3230–3232. https://doi.org/10.1063/1.110207

Hippalgaonkar, K., Wang, Y., Ye, Y., Qiu, D. Y., Zhu, H., Wang, Y., … Zhang, X. (2017). High thermoelectric power factor in two-dimensional crystals of Mo S2. *Physical Review B*, *95*(11), 1–9. https://doi.org/10.1103/PhysRevB.95.115407

Hong, J., Lee, C., Park, J. S., & Shim, J. H. (2016). Control of valley degeneracy in Mo S2 by layer thickness and electric field and its effect on thermoelectric properties. *Physical Review B*, *93*(3), 2–7. https://doi.org/10.1103/PhysRevB.93.035445

Hu, T., Jia, F., Zhao, G., Wu, J., Stroppa, A., & Ren, W. (2018). Intrinsic and anisotropic Rashba spin splitting in Janus transition-metal dichalcogenide monolayers. *Physical Review B*, *97*, 235404. https://doi.org/10.1103/PhysRevB.97.235404

Huang, W., Da, H., & Liang, G. (2013). Thermoelectric performance of MX2 (M Mo,W; X S,Se) monolayers. *Journal of Applied Physics*, *113*(10). https://doi.org/10.1063/1.4794363

Huang, W., Luo, X., Gan, C. K., Quek, S. Y., & Liang, G. (2014). Theoretical study of thermoelectric properties of few-layer MoS2 and WSe2. *Physical Chemistry Chemical Physics*, *16*(22), 10866–10874. https://doi.org/10.1039/c4cp00487f

Huo, N., Yang, S., Wei, Z., Li, S. S., Xia, J. B., & Li, J. (2014). Photoresponsive and Gas Sensing Field-Effect Transistors based on Multilayer WS 2 Nanoflakes. *Scientific Reports*, *4*, 1–9. https://doi.org/10.1038/srep05209

Ibrahim M Abdel-Motaleb, S. M. Q. (2017). Thermoelectric Devices: Principles and Future Trends. *ArXiv [Cond-Mat.Mtrl-Sci]*. https://doi.org/10.1097/00004032-200112000-00023

Jin, C., Tang, X., Tan, X., Smith, S. C., Dai, Y., & Kou, L. (2019). A Janus MoSSe monolayer: a superior and strain-sensitive gas sensing material. *Journal of Materials Chemistry A*, *7*(3), 1099–1106. https://doi.org/10.1039/C8TA08407F

Jin, Z., Liao, Q., Fang, H., Liu, Z., Liu, W., Ding, Z., … Yang, N. (2015). A Revisit to High Thermoelectric Performance of Single-layer MoS2. *Scientific Reports*, *5*(April). https://doi.org/10.1038/srep18342

Johari, P., & Shenoy, V. B. (2012). Tuning the electronic properties of semiconducting transition metal dichalcogenides by applying mechanical strains. *ACS Nano*, *6*(6), 5449–5456. https://doi.org/10.1021/nn301320r

K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, Y. Zhang, S. V. Dubonos, I. V. Grigorieva, A. A. F. (2004). Electric Field Effect in Atomically Thin Carbon Films. *Science*, *306*, 666–670. https://doi.org/10.1126/science.1102896

Kamieniecki, E., Baglio, J. A., Zoski, G. D., Calabrese, G. S., Harrison, D. J., Ricco, A. J., & Wrighton, M. S. (1983). Electrochemical Characterization of p-Type Semiconducting Tungsten Disulfide Photocathodes: Efficient Photoreduction Processes at Semiconductor/Liquid Electrolyte Interfaces. *Journal of the American Chemical Society*, *105*(8), 2246–2256. https://doi.org/10.1021/ja00346a024

Kang, J., Tongay, S., Zhou, J., Li, J., & Wu, J. (2013). Band offsets and heterostructures of two-dimensional semiconductors. *Applied Physics Letters*, *102*(1). https://doi.org/10.1063/1.4774090

Kastner, M. (1972). Bonding bands, lone-pair bands, and impurity states in chalcogenide semiconductors. *Physical Review Letters*, *28*(6), 355–357. https://doi.org/10.1103/PhysRevLett.28.355

Kim, G., Shao, L., Zhang, K., & Pipe, K. P. (2013). Engineered doping of organic semiconductors for enhanced thermoelectric efficiency. *Nature Materials*, *12*(5), 1–5. https://doi.org/10.1038/nmat3635

Kohn, W., & Sham, L. J. (1965a). Self-consistent equations including exchange and correlation effects. *Physical Review*, *140*(4A). https://doi.org/10.1103/PhysRev.140.A1133

Kohn, W., & Sham, L. J. (1965b). Self-consistent equations including exchange and correlation effects. *Physical Review*, *140*(4A), 1133–1138. https://doi.org/10.1103/PhysRev.140.A1133

Kong, H. (2008). Thermoelectric Property Studies on Lead Chalcogenides , Double-filled Cobalt Tri-Antimonide and Rare Earth. *Analysis*.

Kumar, S., & Schwingenschlögl, U. (2015). Thermoelectric response of bulk and monolayer MoSe2 and WSe2. *Chemistry of Materials*, *27*(4), 1278–1284. https://doi.org/10.1021/cm504244b

Kundu, A., Mingo, N., Broido, D. A., & Stewart, D. A. (2011). Role of light and heavy embedded nanoparticles on the thermal conductivity of SiGe alloys. *Physical Review B - Condensed Matter and Materials Physics*, *84*(12), 1–5. https://doi.org/10.1103/PhysRevB.84.125426

L. D. Hicks, M. S. D. (1993). Effect of quantum-well structures on the thermoelectric Bgure of merit. *Phys. Rev. B*, *47*(19), 12727–12731. https://doi.org/10.1177/000306518903700411

Langreth, D. C., & Mehl, M. J. (1983). Beyond the local-density approximation in calculations of ground-state electronic properties. *Physical Review B*, *28*(4), 1809–1834. https://doi.org/10.1103/PhysRevB.28.1809

Lee, C., Hong, J., Whangbo, M. H., & Shim, J. H. (2013). Enhancing the thermoelectric properties of layered transition-metal dichalcogenides 2H-MQ2 (M = Mo, W; Q = S, Se, Te) by layer mixing: Density functional investigation. *Chemistry of Materials*, *25*(18), 3745–3752. https://doi.org/10.1021/cm402281n

Leenaerts, O., Partoens, B., & Peeters, F. M. (2008). Adsorption of H2 O, N H3, CO, N O2, and NO on graphene: A

first-principles study. *Physical Review B - Condensed Matter and Materials Physics*, *77*(12), 1–6. https://doi.org/10.1103/PhysRevB.77.125416

Li, F., Wei, W., Zhao, P., Huang, B., & Dai, Y. (2017). Electronic and Optical Properties of Pristine and Vertical and Lateral Heterostructures of Janus MoSSe and WSSe. *Journal of Physical Chemistry Letters*, *8*(23), 5959–5965. https://doi.org/10.1021/acs.jpclett.7b02841

Li, Hai, Wu, J., Yin, Z., & Zhang, H. (2014). Preparation and applications of mechanically exfoliated single-layer and multilayer MoS2 and WSe2 nanosheets. *Accounts of Chemical Research*, *47*(4), 1067–1075. https://doi.org/10.1021/ar4002312

Li, Hai, Yin, Z., He, Q., Li, H., Huang, X., Lu, G., … Zhang, H. (2012). Fabrication of single- and multilayer MoS 2 film-based field-effect transistors for sensing NO at room temperature. *Small*, *8*(1), 63–67. https://doi.org/10.1002/smll.201101016

Li, Hongxing, Huang, M., & Cao, G. (2016). Markedly different adsorption behaviors of gas molecules on defective monolayer MoS2: A first-principles study. *Physical Chemistry Chemical Physics*, *18*(22), 15110–15117. https://doi.org/10.1039/c6cp01362g

Li, L., Yu, Y., Ye, G. J., Ge, Q., Ou, X., Wu, H., … Zhang, Y. (2014). Black phosphorus field-effect transistors. *Nature Nanotechnology*, *9*(5), 372–377. https://doi.org/10.1038/nnano.2014.35

Li, X. L., Han, W. P., Wu, J. Bin, Qiao, X. F., Zhang, J., & Tan, P. H. (2017). Layer-Number Dependent Optical Properties of 2D Materials and Their Application for Thickness Determination. *Advanced Functional Materials*, *27*(19). https://doi.org/10.1002/adfm.201604468

Liu, G. Bin, Xiao, D., Yao, Y., Xu, X., & Yao, W. (2015). Electronic structures and theoretical modelling of two-dimensional group-VIB transition metal dichalcogenides. *Chemical Society Reviews*, *44*(9), 2643–2663. https://doi.org/10.1039/c4cs00301b

Liu, K. K., Zhang, W., Lee, Y. H., Lin, Y. C., Chang, M. T., Su, C. Y., … Li, L. J. (2012). Growth of large-area and highly crystalline MoS 2 thin layers on insulating substrates. *Nano Letters*, *12*(3), 1538–1544. https://doi.org/10.1021/nl2043612

Liu, N., Kim, P., Kim, J. H., Ye, J. H., Kim, S., & Lee, C. J. (2014). Large-area atomically thin MoS2 nanosheets prepared using electrochemical exfoliation. *ACS Nano*, *8*(7), 6902–6910. https://doi.org/10.1021/nn5016242

Lu, A. Y., Zhu, H., Xiao, J., Chuu, C. P., Han, Y., Chiu, M. H., … Li, L. J. (2017). Janus monolayers of transition metal dichalcogenides. *Nature Nanotechnology*, *12*(8), 744–749. https://doi.org/10.1038/nnano.2017.100

Lv, H. Y., Lu, W. J., Shao, D. F., Lu, H. Y., & Sun, Y. P. (2016). Strain-induced enhancement in the thermoelectric performance of a ZrS2 monolayer. *Journal of Materials Chemistry C*, *4*(20), 4538–4545. https://doi.org/10.1039/c6tc01135g

Lv, H. Y., Lu, W. J., Shao, D. F., & Sun, Y. P. (2014). Enhanced thermoelectric performance of phosphorene by strain-induced band convergence. *Physical Review B - Condensed Matter and Materials Physics*, *90*(8), 1–8. https://doi.org/10.1103/PhysRevB.90.085433

Ma, D., Ma, B., Lu, Z., He, C., Tang, Y., Lu, Z., & Yang, Z. (2017). Interaction between H2O, N2, CO, NO, NO2 and N2O molecules and a defective WSe2 monolayer. *Physical Chemistry Chemical Physics*, *19*(38), 26022–26033. https://doi.org/10.1039/c7cp04351a

Ma, L., Tan, Y., Ghorbani-Asl, M., Boettger, R., Kretschmer, S., Zhou, S., … Chen, F. (2017). Tailoring the optical properties of atomically-thin WS2: Via ion irradiation. *Nanoscale*, *9*(31), 11027–11034. https://doi.org/10.1039/c7nr02025b

Ma, X., Wu, X., Wang, H., & Wang, Y. (2018). A Janus MoSSe monolayer: A potential wide solar-spectrum water-splitting photocatalyst with a low carrier recombination rate. *Journal of Materials Chemistry A*, *6*(5), 2295–2301. https://doi.org/10.1039/c7ta10015a

Madsen, G. K. H., & Singh, D. J. (2006). BoltzTraP. A code for calculating band-structure dependent quantities. *Computer Physics Communications*, *175*(1), 67–71. https://doi.org/10.1016/j.cpc.2006.03.007

Mak, K. F., Lee, C., Hone, J., Shan, J., & Heinz, T. F. (2010). Atomically thin MoS2: A new direct-gap semiconductor. *Physical Review Letters*, *105*(13), 2–5. https://doi.org/10.1103/PhysRevLett.105.136805

Manzeli, S., Ovchinnikov, D., Pasquier, D., Yazyev, O. V., & Kis, A. (2017). 2D transition metal dichalcogenides. *Nature Reviews Materials*, *2*. https://doi.org/10.1038/natrevmats.2017.33

Molina-Sánchez, A., & Wirtz, L. (2011). Phonons in single-layer and few-layer MoS2 and WS2. *Physical Review B - Condensed Matter and Materials Physics*, *84*(15), 1–8. https://doi.org/10.1103/PhysRevB.84.155413

Nan, H., Wang, Z., Wang, W., Liang, Z., Lu, Y., Chen, Q., … Ni, Z. (2014). Strong photoluminescence enhancement of MoS2through defect engineering and oxygen bonding. *ACS Nano*, *8*(6), 5738–5745. https://doi.org/10.1021/nn500532f

Natkaeo, A., Phokharatkul, D., Hodak, J. H., Wisitsoraat, A., & Hodak, S. K. (2018). Highly selective sub–10 ppm H2S gas sensors based on Ag-doped CaCu3Ti4O12 films. *Sensors and Actuators, B: Chemical*, *260*, 571–580. https://doi.org/10.1016/j.snb.2017.12.134

Ni, Z. H., Yu, T., Lu, Y. H., Wang, Y. Y., Feng, Y. P., & Shen, Z. X. (2008). Uniaxial strain on graphene: Raman

spectroscopy study and band-gap opening. *ACS Nano*, *2*(11), 2301–2305. https://doi.org/10.1021/nn800459e
Ni, Z., Liu, Q., Tang, K., Zheng, J., Zhou, J., Qin, R., … Lu, J. (2012). Tunable bandgap in silicene and germanene. *Nano Letters*, *12*(1), 113–118. https://doi.org/10.1021/nl203065e
Niemegeers, A., Burgelman, M., & Decock, K. (2016). Alex Niemegeers, Marc Burgelman, Koen Decock, Johan Verschraegen, Stefaan Degrave Version: 27 june 2015. *SCAPS Manual*, (September).
Omini, M., & Sparavigna, A. (1995). An iterative approach to the phonon Boltzmann equation in the theory of thermal conductivity. *Physica B: Physics of Condensed Matter*, *212*(2), 101–112. https://doi.org/10.1016/0921-4526(95)00016-3
Pack, J. D., & Monkhorst, H. J. (1977). "special points for Brillouin-zone integrations"-a reply. *Physical Review B*, *16*(4), 1748–1749. https://doi.org/10.1103/PhysRevB.16.1748
Pandey, K., Singh, D., Gupta, S. K., Yadav, P., Sonvane, Y., Lukačević, I., … Ahuja, R. (2018). Improving electron transport in the hybrid perovskite solar cells using CaMnO3-based buffer layer. *Nano Energy*, *45*, 287–297. https://doi.org/10.1016/j.nanoen.2018.01.009
Pashangpour, M. (2011). Electronic Structure Calculation of Adsorbate Gas Molecules on a BN Nanolayer , a First Principle Study. *Internation Proceedings of Chemical, Biological & Environmental Engineering*, *2*, 113–116.
Peng, R., Ma, Y., Zhang, S., Huang, B., & Dai, Y. (2018). Valley Polarization in Janus Single-Layer MoSSe via Magnetic Doping [Rapid-communication]. *Journal of Physical Chemistry Letters*, *9*(13), 3612–3617. https://doi.org/10.1021/acs.jpclett.8b01625
Perdew, J. P. (2001). Jacob's ladder of density functional approximations for the exchange-correlation energy. *AIP Conference Proceedings*, *1*(2001), 1–20. https://doi.org/10.1063/1.1390175
Perdew, J. P., Burke, K., & Ernzerhof, M. (1997). Generalized Gradient Approximation Made Simple [Phys. Rev. Lett. 77, 3865 (1996)]. *Physical Review Letters*, *78*(7), 1396–1396. https://doi.org/10.1103/PhysRevLett.78.1396
Petersen, K. E. (1982). Silicon as a Mechanical Material. *Proceedings of the IEEE*, *70*(5), 420–457. https://doi.org/10.1109/PROC.1982.12331
Poudel, B., Hao, Q., Ma, Y., Lan, Y., Minnich, A., Yu, B., … Ren, Z. (2008). High-thermoelectric performance of nanostructured bismuth antimony telluride bulk alloys. *Science*, *320*(5876), 634–638. https://doi.org/10.1126/science.1156446
queksy. (2012). *First Principles Investigations of the Atomic, Electronic, and Thermoelectric Properties of Equilibrium and Strained Bi*. 1–35. https://doi.org/10.1016/j.amjcard.2015.11.031
Ramasubramaniam, A., Naveh, D., & Towe, E. (2011). Tunable band gaps in bilayer transition-metal dichalcogenides. *Physical Review B - Condensed Matter and Materials Physics*, *84*(20), 1–10. https://doi.org/10.1103/PhysRevB.84.205325
Roondhe, B., Patel, K., & Jha, P. K. (2019). Two-dimensional metal carbide comrade for tracing CO and CO2. *Applied Surface Science*, *496*(July), 143685. https://doi.org/10.1016/j.apsusc.2019.143685
Ross, J. S., Wu, S., Yu, H., Ghimire, N. J., Jones, A. M., Aivazian, G., … Xu, X. (2013). Electrical control of neutral and charged excitons in a monolayer semiconductor. *Nature Communications*, *4*, 1–6. https://doi.org/10.1038/ncomms2498
Roy, S., & Bermel, P. (2018). Electronic and optical properties of ultra-thin 2D tungsten disulfide for photovoltaic applications. *Solar Energy Materials and Solar Cells*, *174*(January 2017), 370–379. https://doi.org/10.1016/j.solmat.2017.09.011
Sahoo, M. P. K., Wang, J., Zhang, Y., Shimada, T., & Kitamura, T. (2016). Modulation of Gas Adsorption and Magnetic Properties of Monolayer-MoS2 by Antisite Defect and Strain. *Journal of Physical Chemistry C*, *120*(26), 14113–14121. https://doi.org/10.1021/acs.jpcc.6b03284
Schmidt, H., Giustiniano, F., & Eda, G. (2015a). Electronic transport properties of transition metal dichalcogenide field-effect devices: surface and interface effects. *Chemical Society Reviews*, *44*(21), 7715–7736. https://doi.org/10.1039/c5cs00275c
Schmidt, H., Giustiniano, F., & Eda, G. (2015b). Electronic transport properties of transition metal dichalcogenide field-effect devices: surface and interface effects. *Chemical Society Reviews*, *44*(21), 7715–7736. https://doi.org/10.1039/c5cs00275c
Schutte, W. J., De Boer, J. L., & Jellinek, F. (1987). Crystal structures of tungsten disulfide and diselenide. *Journal of Solid State Chemistry*, *70*(2), 207–209. https://doi.org/10.1016/0022-4596(87)90057-0
Seijas-Bellido, J. A., Rurali, R., Íñiguez, J., Colombo, L., & Melis, C. (2019). Strain engineering of ZnO thermal conductivity. *Physical Review Materials*, *3*(6), 1–8. https://doi.org/10.1103/PhysRevMaterials.3.065401
Sharma, M., Kumar, A., Ahluwalia, P. K., & Pandey, R. (2014). Strain and electric field induced electronic properties of two-dimensional hybrid bilayers of transition-metal dichalcogenides. *Journal of Applied Physics*, *116*(6). https://doi.org/10.1063/1.4892798
Shockley, W., & Queisser, H. J. (1961). Detailed balance limit of efficiency of p-n junction solar cells. *Journal of Applied Physics*, *32*(3), 510–519. https://doi.org/10.1063/1.1736034

Shuai, J., Mao, J., Song, S., Zhu, Q., Sun, J., Wang, Y., … Ren, Z. (2017). Tuning the carrier scattering mechanism to effectively improve the thermoelectric properties. *Energy and Environmental Science*, *10*(3), 799–807. https://doi.org/10.1039/c7ee00098g

Singh, E., Kim, K. S., Yeom, G. Y., & Nalwa, H. S. (2017). Two-dimensional transition metal dichalcogenide-based counter electrodes for dye-sensitized solar cells. *RSC Advances*, *7*(45), 28234–28290. https://doi.org/10.1039/c7ra03599c

Snyder, G. J., & Snyder, A. H. (2017). Figure of merit ZT of a thermoelectric device defined from materials properties. *Energy and Environmental Science*, *10*(11), 2280–2283. https://doi.org/10.1039/c7ee02007d

Sommerhalter, C., Matthes, T. W., Boneberg, J., Lux-Steiner, M. C., & Leiderer, P. (1999). Investigation of acceptors in p-type WS2by standard and photo-assisted scanning tunneling microscopy/spectroscopy. *Applied Surface Science*, *144–145*, 564–569. https://doi.org/10.1016/S0169-4332(98)00866-6

Song, J., & Lou, H. (2018). Improvement of gas-adsorption performances of Ag-functionalized monolayer MoS2 surfaces: A first-principles study. *Journal of Applied Physics*, *123*(17). https://doi.org/10.1063/1.5022829

Soni, H., & Jha, P. K. (2015). Ab-initio study of dynamical properties of two dimensional MoS2 under strain. *AIP Advances*, *5*(10), 1–7. https://doi.org/10.1063/1.4932974

Subhash L. Shindé, G. P. S. (2014). *Length-Scale Dependent Phonon Interactions*.

Sun, J., Remsing, R. C., Zhang, Y., Sun, Z., Ruzsinszky, A., Peng, H., … Perdew, J. P. (2016). Accurate first-principles structures and energies of diversely bonded systems from an efficient density functional. *Nature Chemistry*, *8*(9), 831–836. https://doi.org/10.1038/nchem.2535

Tani, J. I., & Kido, H. (2007). Thermoelectric properties of P-doped Mg2Si semiconductors. *Japanese Journal of Applied Physics, Part 1: Regular Papers and Short Notes and Review Papers*, *46*(6 A), 3309–3314. https://doi.org/10.1143/JJAP.46.3309

Tasker, P. W. (1996). Generalized Gradient Approximation Made Simple John. *Physical Review Letters*, *77*(18), 3865–3868. https://doi.org/10.1103/PhysRevLett.77.3865

Thilagam, A. (2017). Transition-metal dichalcogenide heterostructure solar cells: a numerical study. *Journal of Mathematical Chemistry*, *55*(1), 50–64. https://doi.org/10.1007/s10910-016-0669-9

Togo, A., Chaput, L., & Tanaka, I. (2015). Distributions of phonon lifetimes in Brillouin zones. *Physical Review B - Condensed Matter and Materials Physics*, *91*(9). https://doi.org/10.1103/PhysRevB.91.094306

Togo, A., & Tanaka, I. (2015). First principles phonon calculations in materials science. *Scripta Materialia*, *108*, 1–5. https://doi.org/10.1016/j.scriptamat.2015.07.021

Tongay, S., Suh, J., Ataca, C., Fan, W., Luce, A., Kang, J. S., … Wu, J. (2013). Defects activated photoluminescence in two-dimensional semiconductors: Interplay between bound, charged, and free excitons. *Scientific Reports*, *3*, 1–5. https://doi.org/10.1038/srep02657

Torbatian, Z., & Asgari, R. (2018). Plasmonic physics of 2D crystalline materials. *Applied Sciences (Switzerland)*, *8*(2). https://doi.org/10.3390/app8020238

Toriumi, A., Iwase, M., & Tango, H. (1994). On the Universality of Inversion Layer Mobility in Si MOSFET's: Part I—Effects of Substrate Impurity Concentration. *IEEE Transactions on Electron Devices*, *41*(12), 2357–2362. https://doi.org/10.1109/16.337449

Tran, F., & Blaha, P. (2009). Accurate band gaps of semiconductors and insulators with a semilocal exchange-correlation potential. *Physical Review Letters*, *102*(22), 5–8. https://doi.org/10.1103/PhysRevLett.102.226401

Wang, Yun, Yeow, J. T. W. (2009). A review of carbon nanotubes-based gas sensors. *Journal of Sensors*, *2009*. https://doi.org/10.1155/2009/493904

Wang, C., Yin, L., Zhang, L., Xiang, D., & Gao, R. (2010). Metal oxide gas sensors: Sensitivity and influencing factors. *Sensors*, *10*(3), 2088–2106. https://doi.org/10.3390/s100302088

Wang, F., Wang, J., Guo, S., Zhang, J., Hu, Z., & Chu, J. (2017). Tuning Coupling Behavior of Stacked Heterostructures Based on MoS2, WS2, and WSe2. *Scientific Reports*, *7*(February), 1–10. https://doi.org/10.1038/srep44712

Wang, Q. H., Kalantar-Zadeh, K., Kis, A., Coleman, J. N., & Strano, M. S. (2012). Electronics and optoelectronics of two-dimensional transition metal dichalcogenides. *Nature Nanotechnology*, *7*(11), 699–712. https://doi.org/10.1038/nnano.2012.193

Wang, T., Zhao, R., Zhao, X., An, Y., Dai, X., & Xia, C. (2016). Tunable donor and acceptor impurity states in a WSe2 monolayer by adsorption of common gas molecules. *RSC Advances*, *6*(86), 82793–82800. https://doi.org/10.1039/c6ra17643g

Wen, Y. U., Debbarma, R., Nguyen, P., Che, S., Deng, S., Seacrist, M. R., & Berry, V. (2017). WS 2 /Silicon Heterojunction Solar Cells. *Ieee Nanotechnology Magazine*, (April), 2–8.

Wickramaratne, D., Zahid, F., & Lake, R. K. (2014a). Electronic and thermoelectric properties of few-layer transition metal dichalcogenides. *Journal of Chemical Physics*, *140*(12). https://doi.org/10.1063/1.4869142

Wickramaratne, D., Zahid, F., & Lake, R. K. (2014b). Electronic and thermoelectric properties of few-layer transition metal dichalcogenides. *Journal of Chemical Physics*, *140*(12). https://doi.org/10.1063/1.4869142

Wood, J. D., Wells, S. A., Jariwala, D., Chen, K., Cho, E., Sangwan, V. K., … Hersam, M. C. (2014). Effective Passivation of Exfoliated Black Phosphorus Transistors against Ambient Degradation. *Nano Letters*, 1–7. https://doi.org/10.1021/nl5032293

Woomer, A. H., Farnsworth, T. W., Hu, J., Wells, R. A., Donley, C. L., & Warren, S. C. (2015). Phosphorene: Synthesis, Scale-Up, and Quantitative Optical Spectroscopy. *ACS Nano*, *9*(9), 8869–8884. https://doi.org/10.1021/acsnano.5b02599

Xiang, J., Ali, R. N., Yang, Y., Zheng, Z., Xiang, B., & Cui, X. (2019). Monolayer MoS 2 thermoelectric properties engineering via strain effect. *Physica E: Low-Dimensional Systems and Nanostructures*, *109*(398), 248–252. https://doi.org/10.1016/j.physe.2019.01.029

Xiao, J., Long, M., Li, X., Zhang, Q., Xu, H., & Chan, K. S. (2014). Effects of van der Waals interaction and electric field on the electronic structure of bilayer MoS 2. *Journal of Physics Condensed Matter*, *26*(40). https://doi.org/10.1088/0953-8984/26/40/405302

Yang, G., Yan, P., Zhu, C., Gu, Y., Lu, N., Xue, J., … Fang, X. (2019). Selenium Vacancy–Enhanced Gas Adsorption of Monolayer Hafnium Diselenide (HfSe 2) from a Theoretical Perspective . *Advanced Theory and Simulations*, *2*(7), 1900052. https://doi.org/10.1002/adts.201900052

Yin, W. J., Wen, B., Nie, G. Z., Wei, X. L., & Liu, L. M. (2018). Tunable dipole and carrier mobility for a few layer Janus MoSSe structure. *Journal of Materials Chemistry C*, *6*(7), 1693–1700. https://doi.org/10.1039/c7tc05225a

Yu, X., & Sivula, K. (2016). Toward Large-Area Solar Energy Conversion with Semiconducting 2D Transition Metal Dichalcogenides. *ACS Energy Letters*, *1*(1), 315–322. https://doi.org/10.1021/acsenergylett.6b00114

Yuan, K., Zhang, X., Li, L., & Tang, D. (2019). Effects of tensile strain and finite size on thermal conductivity in monolayer WSe2. *Physical Chemistry Chemical Physics*, *21*(1), 468–477. https://doi.org/10.1039/c8cp06414h

Yuan, S., Roldán, R., Katsnelson, M. I., & Guinea, F. (2014). *Effect of Point Defects on the Optical and Transport Properties of MoS2 and WS2*. 1–9. https://doi.org/10.1103/PhysRevB.90.041402

Yue, Q., Shao, Z., Chang, S., & Li, J. (2013). Adsorption of gas molecules on monolayer MoS2 and effect of applied electric field. *Nanoscale Research Letters*, *8*(1), 425. https://doi.org/10.1186/1556-276X-8-425

Zaporotskova, I. V., Boroznina, N. P., Parkhomenko, Y. N., & Kozhitov, L. V. (2016). Carbon nanotubes: Sensor properties. A review. *Modern Electronic Materials*, *2*(4), 95–105. https://doi.org/10.1016/j.moem.2017.02.002

Zeng, F., Zhang, W.-B., & Tang, B.-Y. (2015). The electronic structure and elastic property of monolayer and bilayer transition metal dichalcogenides MX$_2$ (M=Mo,W;X=O,S,Se,Te): A comparative first-principles study. *Chinese Physics B*, *24*(9), 097103. https://doi.org/10.1088/1674-1056/24/9/097103

Zeng, Z., Sun, T., Zhu, J., Huang, X., Yin, Z., Lu, G., … Zhang, H. (2012). An effective method for the fabrication of few-layer-thick inorganic nanosheets. *Angewandte Chemie - International Edition*, *51*(36), 9052–9056. https://doi.org/10.1002/anie.201204208

Zhang, C., Li, A., Zhao, Y. H., Bai, S. L., & Zhang, Y. F. (2018). Thermal, electrical and mechanical properties of graphene foam filled poly(methyl methacrylate) composite prepared by in situ polymerization. *Composites Part B: Engineering*, *135*(October 2017), 201–206. https://doi.org/10.1016/j.compositesb.2017.10.026

Zhang, Jian, Qin, Z., Zeng, D., & Xie, C. (2017). Metal-oxide-semiconductor based gas sensors: Screening, preparation, and integration. *Physical Chemistry Chemical Physics*, *19*(9), 6313–6329. https://doi.org/10.1039/c6cp07799d

Zhang, Jing, Jia, S., Kholmanov, I., Dong, L., Er, D., Chen, W., … Lou, J. (2017). Janus Monolayer Transition-Metal Dichalcogenides. *ACS Nano*, *11*(8), 8192–8198. https://doi.org/10.1021/acsnano.7b03186

Zhang, X., Qiao, X. F., Shi, W., Wu, J. Bin, Jiang, D. S., & Tan, P. H. (2015). Phonon and Raman scattering of two-dimensional transition metal dichalcogenides from monolayer, multilayer to bulk material. *Chemical Society Reviews*, *44*(9), 2757–2785. https://doi.org/10.1039/c4cs00282b

Zhao, B., Li, C. Y., Liu, L. L., Zhou, B., Zhang, Q. K., Chen, Z. Q., & Tang, Z. (2016). Adsorption of gas molecules on Cu impurities embedded monolayer MoS 2 : A first- principles study. *Applied Surface Science*, *382*(2), 280–287. https://doi.org/10.1016/j.apsusc.2016.04.158

Zhao, L. D., Tan, G., Hao, S., He, J., Pei, Y., Chi, H., … Kanatzidis, M. G. (2016). Ultrahigh power factor and thermoelectric performance in hole-doped single-crystal SnSe. *Science*, *351*(6269), 141–144. https://doi.org/10.1126/science.aad3749

Zhao, W., Ghorannevis, Z., Amara, K. K., Pang, J. R., Toh, M., Zhang, X., … Eda, G. (2013). Lattice dynamics in mono- and few-layer sheets of WS2 and WSe2. *Nanoscale*, *5*(20), 9677–9683. https://doi.org/10.1039/c3nr03052k

Zhao, Z. Y., & Liu, Q. L. (2018). Study of the layer-dependent properties of MoS2 nanosheets with different crystal structures by DFT calculations. *Catalysis Science and Technology*, *8*(7), 1867–1879. https://doi.org/10.1039/c7cy02252b

Zhou, C., Yang, W., & Zhu, H. (2015). Mechanism of charge transfer and its impacts on Fermi-level pinning for gas molecules adsorbed on monolayer WS2. *Journal of Chemical Physics*, *142*(21).

https://doi.org/10.1063/1.4922049
Zhou, H., Wang, C., Shaw, J. C., Cheng, R., Chen, Y., Huang, X., … Duan, X. (2015). Large area growth and electrical properties of p-type WSe2atomic layers. *Nano Letters*, *15*(1), 709–713. https://doi.org/10.1021/nl504256y
Zhou, W., Zou, X., Najmaei, S., Liu, Z., Shi, Y., Kong, J., … Idrobo, J. C. (2013a). Intrinsic structural defects in monolayer molybdenum disulfide. *Nano Letters*, *13*(6), 2615–2622. https://doi.org/10.1021/nl4007479
Zhou, W., Zou, X., Najmaei, S., Liu, Z., Shi, Y., Kong, J., … Idrobo, J. C. (2013b). Intrinsic structural defects in monolayer molybdenum disulfide. *Nano Letters*, *13*(6), 2615–2622. https://doi.org/10.1021/nl4007479
Ziman, J. M., & Levy, P. W. (2001). Electrons and phonons: the theory of transport phenomena in solids. In *Oxford University Press*. https://doi.org/10.1063/1.3057244
Zou, D., Xie, S., Liu, Y., Lin, J., & Li, J. (2013). Electronic structures and thermoelectric properties of layered BiCuOCh oxychalcogenides (Ch = S, Se and Te): First-principles calculations. *Journal of Materials Chemistry A*, *1*(31), 8888–8896. https://doi.org/10.1039/c3ta11222e