

DAFTAR PUSTAKA

- Born, M., & Huang, K. (1954). *Dynamical theory of crystal lattices*. Oxford University Press.
- 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.
- Chen, A., & Luo, X. (2023). First-principles investigation of possible room-temperature topological insulators in monolayers. *RSC Advances*, 13(43), 31375–31385.
- Cheng, M., Chen, H., & Chen, J. (2024). Regulating Anderson localization with defect disorder. *Chinese Physics B*.
- Ciftci, Y. O., Colakoglu, K., & Deligoz, E. (2008). A first-principles study on TlX (X = P, As). *Central European Journal of Physics*, 6(4), 802–807.
- Dahham, O. S., Al-Zamili, K., & Zulkepli, N. N. (2024). A Review on Common Approaches Used for Graphene Characterization. In *Journal of Al-Farabi For Engineering Sciences*.
- Daoud, S. (2017). Thermal properties of cubic zincblende thallium-phosphide from quasi-harmonic Debye model approximation. *International Journal of Physical Research*, 5(1), 14–16.
- Daoud, S., & Bioud, N. (2014). Structural properties of (B3) TIP under pressure. *International Journal of Physical Research*, 2(2), 50–55.
- Eisberg, R. M., & Resnick, R. (1985). *Quantum physics of atoms, molecules, solids, nuclei, and particles* (2nd ed.). Wiley.
- Griffiths, D. J. (2005). *Introduction to quantum mechanics* (2nd ed.). Pearson Prentice Hall.
- Hamann, D. R., Schluter, M., & Chiang, C. (1979). Norm-conserving pseudopotentials. *Physical Review Letters*, 43(20), 1494–1497.
- Hartree, D. R. (1928). The wave mechanics of an atom with a non-Coulomb central field. Part I: Theory and methods. *Mathematical Proceedings of the Cambridge Philosophical Society*, 24(1), 89–110.
- Herring, C. (1933). A new method for calculating wave functions in crystals. *Physical Review*, 43(2), 103–113.

- Hess, P. (2021). Bonding, structure, and mechanical stability of 2D materials: The predictive power of the periodic table. *Nanoscale Horizons*, 6(11), 856–892.
- Heyd, J., Scuseria, G. E., & Ernzerhof, M. (2003). Hybrid functionals based on a screened Coulomb potential. *Journal of Chemical Physics*, 118(18), 8207–8215.
- Hohenberg, P., & Kohn, W. (1964). Inhomogeneous electron gas. *Physical Review*, 136(3B), B864–B871.
- Jian Cai, Ruffieux, P., Jaafar, R., Bieri, M., Braun, T., Blankenburg, S., ... Fasel, R. (2014). *Atomically precise bottom-up fabrication of graphene nanoribbons*. *Nature*, 466, 470–473.
- Karmakar, S., Biswas, R., & Saha-Dasgupta, T. (2023). Giant Rashba effect and nonlinear anomalous Hall conductivity in a two-dimensional molybdenum-based Janus structure. *Physical Review B*, 107, 075403.
- Karmakar, S., Kundu, S. K., & Taki, G. S. (2021). Bandgap study of defect-induced graphene structures. In *Proceedings of the 5th International Conference on Electronics, Materials Engineering & Nano-Technology (IEMENTech)* (pp. 1–3). IEEE.
- Kittel, C. (2005). *Introduction to solid state physics* (8th ed.). John Wiley & Sons.
- Kleinman, L., & Bylander, D. M. (1982). Efficacious form for model pseudopotentials. *Physical Review Letters*, 48(20), 1425–1428.
- Kohn, W. (1999). Nobel lecture: Electronic structure of matter—Wave functions and density functionals. *Reviews of Modern Physics*, 71(5), 1253–1266.
- Koukaras, E. N., Kalosakas, G., Galiotis, C., & Papagelis, K. (2015). Phonon properties of graphene derived from molecular dynamics simulations. *Scientific Reports*, 5, 12923.
- Lewars, E. G. (2016). Introduction to quantum mechanics in computational chemistry. In *Computational chemistry* (pp. 101–191). Springer.
- Martinez, J., 2017, ‘The Hartree-Fock method: from self-consistency to correct symmetry’, *Annalen der Physik*, 529(1–2).
- Merabet, M., Djoudi, L., Sayah, M., Benalia, S., & Rached, D. (2018). Band gap behavior of thallium phosphide and gallium phosphide binary compounds

- and $\text{Ga}_x\text{Tl}_{1-x}\text{P}$ ternary alloys. *Journal of Physics: Conference Series*, 1081(1), 012011.
- Misra, P. K. (2010). *Physics of condensed matter*. Academic Press.
- Nie, Y., Rahman, M., Wang, D., Wang, C., & Guo, G. (201). *Strain-induced topological phase transitions in monolayer honeycomb structures of group-V binary compounds*. *Scientific Reports*, 5, 17980.
- Novoselov, K. S., Geim, A. K., Morozov, S. V., Jiang, D., Zhang, Y., Dubonos, S. V., Grigorieva, I. V, & Firsov, A. A. (2004). Electric Field Effect in Atomically Thin Carbon Films. *Science*, 306 (5696), 666–669.
- Perdew, J. P., & Zunger, A. (1981). Self-interaction correction to density-functional approximations for many-electron systems. *Physical Review B*, 23(10), 5048–5079.
- Perdew, J. P., Burke, K., & Ernzerhof, M. (1996). Generalized gradient approximation made simple. *Physical Review Letters*, 77(18), 3865–3868.
- Şahin, H. (2009). Monolayer honeycomb structures of group-IV elements and III–V binary compounds: First-principles calculations. *Physical Review B*, 80(15), 155453.
- Saidi-Houat, N., Zaoui, A., & Ferhat, M. (2007). Structural stability of thallium–V compounds. *Journal of Physics: Condensed Matter*, 19(10), 106221.
- Schwerdtfeger, P. (2011). The pseudopotential approximation in electronic structure theory. *ChemPhysChem*, 12(17), 3143–3155.
- Sholihun, Kadarisman, H. P., & Nurwantoro, P. (2018). Density-functional theory calculations of formation energy of nitrogen-doped diamond. *Indonesian Journal of Chemistry*, 18(4), 749–754.
- Sholihun. (2015). *First-principles calculations of vacancies in semiconductors* (Doctoral dissertation).
- Sholihun, S., Purnawati, D., Bermundo, J. P., Prayogi, H., Fatomi, Z. S., & Hidayati, S. (2023). Novel two-dimensional square-structured diatomic group-IV materials: the first-principles prediction. *Physica Scripta*, 98(11).
- Sholl, D. S., & Steckel, J. A. (2009). What is density functional theory? In *Density functional theory* (pp. 1–33). Wiley.

- Slater, J. C. (1951). A simplification of the Hartree–Fock method. *Physical Review*, 81(3), 385–390.
- Pawel Spiewak, J., Kurzydłowski, K. J., & others. (2011). *First-principles study of structural and electronic properties of semiconductors*.
- Tully, J. C. (2000). Perspective on “Zur Quantentheorie der Molekeln”. *Theoretical Chemistry Accounts*, 103(3–4), 173–176.
- Wei, Y., Lan, C., Zhou, S., & Li, C. (2023). Recent advances in photodetectors based on two-dimensional material/Si heterojunctions. *Applied Sciences*, 13(19), 11037.
- Young-Woo Son, Cohen, M. L., & Louie, S. G. (2006). *Energy gaps in graphene nanoribbons*. *Physical Review Letters*, 97, 216803.
- Yuan, J. H. (2019). TIPs: An unexplored direct band gap 2D semiconductor with ultra-high carrier mobility. *Journal of Materials Chemistry C*, 7, 639–644.
- Yue, Z., Wang, X., & Gu, M. (2019). Topological insulator materials for advanced optoelectronic devices. In H. Luo (Ed.), *Advanced topological insulators* (pp. 45–70). Wiley & Scrivener.
- Zhang, L., Yu, J., Yang, M., Xie, Q., Peng, H., & Liu, Z. (2017). Band gap engineering of graphene. *Nature Communications*, 4, 1443.
- Zhao, Y. (2022). Pressure-induced superconductivity extending across the topological phase transition in thallium-based topological materials. *Cell Reports Physical Science*, 3(10), 101094.
- Zhou, D. W., Liu, J. S., Peng, P., Chen, L., & Hu, Y. J. (2008). A first-principles study on the structural stability of Al₂Ca, Al₄Ca, and Mg₂Ca phases. *Materials Letters*, 62(2), 206–210.