

DAFTAR PUSTAKA

- Agostini, F. & Curchod, B.F.E., 2022, 'Chemistry without the Born-Oppenheimer approximation.', *Philosophical transactions. Series A, Mathematical, physical, and engineering sciences*, 380(2223), 20200375.
- Almashhadani, H.A., 2014, *Corrosion and Corrosion Protection Studies of Carbon Steel alloy in Seawater using; Zirconia, Silicon Carbide and Alumina Nanoparticles* – PhD thesis .
- Bechstedt, F., Furthmüller, J., Grossner, U. & Raffy, C., 2004, 'Zero- and Two-Dimensional Native Defects', in H. and P.G. Choyke W. J. and Matsunami (ed.), *Silicon Carbide: Recent Major Advances*, pp. 3–25, Springer Berlin Heidelberg, Berlin, Heidelberg.
- Chabi, S., Guler, Z., Brearley, A.J., Benavidez, A.D. & Luk, T.S., 2021a, 'The Creation of True Two-Dimensional Silicon Carbide', *Nanomaterials*, 11(7), 1799.
- Chabi, S., Guler, Z., Brearley, A.J., Benavidez, A.D. & Luk, T.S., 2021b, 'The creation of true two-dimensional silicon carbide', *Nanomaterials*, 11(7).
- Chabi, S. & Kadel, K., 2020, 'Two-Dimensional Silicon Carbide: Emerging Direct Band Gap Semiconductor', *Nanomaterials*, 10(11), 2226.
- Chadi, D.J. & Chang, K.J., 1988, 'Magic numbers for vacancy aggregation in crystalline Si', *Physical Review B*, 38(2), 1523–1525.
- Chaussende, D. & Ohtani, N., 2019, 'Silicon carbide', *Single Crystals of Electronic Materials*, pp. 129–179, Elsevier.
- Chen, X., Yang, X., Xie, X., Peng, Y., Xiao, L., Shao, C., Li, H., Hu, X. & Xu, X., 2023, 'Research progress of large size SiC single crystal materials and devices', *Light: Science & Applications*, 12(1), 28.
- Fatomi, Z.S., Nugraheni, A.D. & Sholihun, 2022, 'Vibrational effect on vacancy concentration in diamond: The density-functional-theory calculation', *Computational Condensed Matter*, 32, e00708.

- Griffiths, David J., 2005, *Introduction to quantum mechanics (2nd ed.)*, Upper Saddle River, NJ : Pearson Prentice Hall.
- 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.
- Hastuti, D.P., Amalia, W., Priska, Z., Nurwantoro, P. & Sholihun, 2020, 'First-principles density-functional-theory calculations of formation and dissociation energies in germanene multivacancies', *Materials Today Communications*, 22, 100754.
- Hoat, D.M., Naseri, M., Hieu, N.N., Ponce-Pérez, R., Rivas-Silva, J.F. & Coccoletzi, G.H., 2020, 'Transition from indirect to direct band gap in SiC monolayer by chemical functionalization: A first principles study', *Superlattices and Microstructures*, 137, 106320.
- Hohenberg, P. & Kohn, W., 1964, 'Inhomogeneous Electron Gas', *Physical Review*, 136(3B), B864–B871.
- Ibele, L.M., Curchod, B.F.E. & Agostini, F., 2022, 'A Photochemical Reaction in Different Theoretical Representations', *The Journal of Physical Chemistry A*, 126(7), 1263–1281.
- Iwata, J.-I., Shinei, C. & Oshiyama, A., 2016, 'Density-functional study of atomic and electronic structures of multivacancies in silicon carbide', *Physical Review B*, 93(12), 125202.
- Karmakar, S., Kundu, S.K. & Taki, G.S., 2021, *Bandgap Study of Defect Induced Graphene Structures, 2021 5th International Conference on Electronics, Materials Engineering & Nano-Technology (IEMENTech)*, 1–3, IEEE.
- Kimoto, T. & Watanabe, H., 2020, 'Defect engineering in SiC technology for high-voltage power devices', *Applied Physics Express*, 13(12), 120101.
- Kimoto, Tsunenobu. & Cooper, J.A., 2014, *Fundamentals of Silicon Carbide Technology : Growth, Characterization, Devices and Applications.*, Wiley.
- Kohn, W., 1999, 'Nobel Lecture: Electronic structure of matter—wave functions and density functionals', *Reviews of Modern Physics*, 71(5), 1253–1266.

- Kohn, W. & Sham, L.J., 1965, ‘Self-Consistent Equations Including Exchange and Correlation Effects’, *Physical Review*, 140(4A), A1133–A1138.
- Koukaras, E.N., Kalosakas, G., Galiotis, C. & Papagelis, K., 2015, ‘Phonon properties of graphene derived from molecular dynamics simulations’, *Scientific Reports*, 5(1), 12923.
- Langpoklakpam, C., Liu, A.-C., Chu, K.-H., Hsu, L.-H., Lee, W.-C., Chen, S.-C., Sun, C.-W., Shih, M.-H., Lee, K.-Y. & Kuo, H.-C., 2022, ‘Review of Silicon Carbide Processing for Power MOSFET’, *Crystals*, 12(2), 245.
- Lewars, E.G., 2016, ‘Introduction to Quantum Mechanics in Computational Chemistry’, *Computational Chemistry*, pp. 101–191, Springer International Publishing, Cham.
- Liu, X., Choi, M.S., Hwang, E., Yoo, W.J. & Sun, J., 2022, ‘Fermi Level Pinning Dependent 2D Semiconductor Devices: Challenges and Prospects’, *Advanced Materials*, 34(15).
- Manju, M.S., Thomas, S., Lee, S.U. & Kulangara Madam, A., 2021, ‘Mechanically robust, self-healing graphene like defective SiC: A prospective anode of Li-ion batteries’, *Applied Surface Science*, 541, 148417.
- Martin Eisberg, R. & Resnick, R., 1985, *Quantum Physics of Atoms, Molecules, Solids, Nuclei, and Particles*, 2nd ed.
- Martinez, J., 2017, ‘The Hartree-Fock method: from self-consistency to correct symmetry’, *Annalen der Physik*, 529(1–2).
- Meng, F., Ma, J., He, J. & Li, W., 2019, ‘Phonon-limited carrier mobility and temperature-dependent scattering mechanism of SiC from first principles’, *Physical Review B*, 99(4), 045201.
- Perdew, J.P., Burke, K. & Ernzerhof, M., 1996, ‘Generalized Gradient Approximation Made Simple’, *Physical Review Letters*, 77(18), 3865–3868.
- Perdew, J.P. & Zunger, A., 1981, ‘Self-interaction correction to density-functional approximations for many-electron systems’, *Physical Review B*, 23(10), 5048–5079.

- Powell, R.C., 2010a, 'Symmetry in Solids', in R.C. Powell (ed.), *Symmetry, Group Theory, and the Physical Properties of Crystals*, pp. 1–24, Springer New York, New York, NY.
- Powell, R.C., 2010b, 'Group Theory', *Symmetry, Group Theory, and the Physical Properties of Crystals*, pp. 25–53, Springer New York, New York, NY.
- Purnawati, D., Fajariah, N., Prayogi, H., Bermundo, J.P. & Nugraheni, A.D., 2023, 'Dissociation-energy calculations of C-multivacancies in diamond: the density-functional-theory study', *Japanese Journal of Applied Physics*, 62(5), 051002.
- Sholihun, 2015, *First-principles Calculations of Vacancies in Semiconductors* 半導体中原子空孔の第一原理計算 Sholihun 1 2 2 3 1 0 2 0 0 9 – PhD thesis .
- Scherrer, A., Agostini, F., Sebastiani, D., Gross, E.K.U. & Vuilleumier, R., 2017, 'On the Mass of Atoms in Molecules: Beyond the Born-Oppenheimer Approximation', *Physical Review X*, 7(3), 031035.
- Sholihun, Amalia, W., Hastuti, D.P., Nurwantoro, P., Nugraheni, A.D. & Budhi, R.H.S., 2019, 'Magic vacancy-numbers in h-BN multivacancies: The first-principles study', *Materials Today Communications*, 20, 100591.
- 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), 115903.
- Sholl, D.S. & Steckel, J.A., 2009, 'What is Density Functional Theory?', *Density Functional Theory*, pp. 1–33, Wiley.
- Singh, A., Mahamiya, V. & Shukla, A., 2023, 'Defect-driven tunable electronic and optical properties of two-dimensional silicon carbide', *Physical Review B*, 108(23), 235311.
- Slater, J.C., 1951, 'A Simplification of the Hartree-Fock Method', *Physical Review*, 81(3), 385–390.
- Slater, J.C., 1953, 'A Generalized Self-Consistent Field Method', *Physical Review*, 91(3), 528–530.

- Sutcliffe, B.T., 1992, 'The Born-Oppenheimer Approximation', in G.H.F. Wilson Stephen and Diercksen (ed.), *Methods in Computational Molecular Physics*, pp. 19–46, Springer US, Boston, MA.
- Tully, J.C., 2000, 'Perspective on "Zur Quantentheorie der Molekeln"', *Theoretical Chemistry Accounts: Theory, Computation, and Modeling (Theoretica Chimica Acta)*, 103(3–4), 173–176.
- Xu, M., Girish, Y.R., Rakesh, K.P., Wu, P., Manukumar, H.M., Byrappa, S.M., Udayabhanu & Byrappa, K., 2021, 'Recent advances and challenges in silicon carbide (SiC) ceramic nanoarchitectures and their applications', *Materials Today Communications*, 28, 102533.
- Zettili, N., 2009, *Quantum mechanics: Concepts and applications*, John Willey and Sons, Jacksonville, USA.