

DAFTAR PUSTAKA

- Androulidakis, C., Kotsidi, M., Gorgolis, G., Pavlou, C., Sygellou, L., Paterakis, G., Koutroumanis, N., dan Galiotis, C., 2021, Multi-functional 2D hybrid aerogels for gas absorption applications, *Scientific reports*, Vol. 11, no. 1, pp 13548
- Atkins, P., 2024, *Concepts in physical chemistry*, Royal Society of Chemistry, Cambridge, England
- Baachaoui, S., Aldulaijan, S., Sementa, L., Fortunelli, A., Dhouib, A., dan Raouafi, N., 2021, Density Functional Theory Investigation of Graphene Functionalization with Activated Carbenes and Its Application in the Sensing of Heavy Metallic Cations, *The Journal of Physical Chemistry C*, Vol. 125, no. 48, pp 26418–26428
- Brémond, É., Pérez-Jiménez, Á. J., Adamo, C., dan Sancho-Garcia, J.-C., 2026, Contemporary DFT: learning from traditional and recent trends for the development and assessment of accurate exchange-correlation functionals, *Physical Chemistry Chemical Physics*, Advance Access published 2026: doi:10.1039/d5cp03373j
- van den Broek, J., Klein Cerrejon, D., Pratsinis, S. E., dan Güntner, A. T., 2020, Selective Formaldehyde Detection at Ppb in Indoor Air with a Portable Sensor, *Journal of Hazardous Materials*, Vol. 399
- Carl, R., 2024, Safety Data Sheet: Acetaldehyde, Advance Access published 2024
- Chaudhary, S. K., Chaudhary, N., Chaudhary, R., dan Chaudhary, N. K., 2022, Review on benefits, toxicity, challenges, and future of graphene-based face masks in the prevention of COVID-19 pandemic, *PeerJ Materials Science*, Vol. 4, pp e20
- Chen, C., Avila, J., Wang, S., Yang, R., Zhang, G., dan Asensio, M. C., 2017, Electronic structure of graphene/hexagonal boron nitride heterostructure revealed by Nano-ARPES, dalam *Journal of Physics: Conference Series*, Institute of Physics Publishing
- Cramer, C. J. ., 2013, *Essentials of computational chemistry : theories and models*, Wiley
- Fang, L., Liu, N., Liu, W., Mo, J., Zhao, Z., Kan, H., Deng, F., Huang, C., Zhao, B., Zeng, X., Sun, Y., Qian, H., Sun, C., Guo, J., dkk., 2022, Indoor Formaldehyde Levels in Residences, Schools, and Offices in China in the Past 30 Years: A Systematic Review, *Indoor Air*, Vol. 32, no. 10
- Giannozzi, P., Baroni, S., Bonini, N., Calandra, M., Car, R., Cavazzoni, C., Ceresoli, D., Chiarotti, G. L., Cococcioni, M., Dabo, I., Dal Corso, A., de Gironcoli, S., Fabris, S., Fratesi, G., dkk., 2009, QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials, *Journal of Physics: Condensed Matter*, Vol. 21, no. 39, pp 395502
- Hassan, I. Z., Kadhém, H. A., dan Mohammed, A. H. S., 2023, DFT Study of Hexagonal Boron Nitride Electronic Properties Using Different Types of

- Exchange Correlation Functionals, *Indian Journal of Pure & Applied Physics*, Advance Access published 2023: doi:10.56042/ijpap.v61i10.2805
- Jung, J., Dasilva, A. M., Macdonald, A. H., dan Adam, S., 2015, Origin of band gaps in graphene on hexagonal boron nitride, *Nature Communications*, Vol. 6
- Kajian, (, Tentang, T., Struktur, S., Keadaan, K., Struktur, D., Grafin, J., Tunggal, L., Lapisan, D., Nurhafizah,), Disa, M., Malakar, H., dan Abdullah, N., 2022, DFT STUDY ON STRUCTURAL PROPERTIES, DENSITY OF STATES AND BAND STRUCTURE OF MONOLAYER & BILAYER GRAPHENE:, diakses pada Malaysian Journal of Analytical Sciences
- Liu, M., Gopakumar, A., Hegde, V. I., He, J., dan Wolverton, C., 2024, High-Throughput hybrid-functional DFT calculations of bandgaps and formation energies and multifidelity learning with uncertainty quantification, *Physical Review Materials*, Vol. 8, no. 4
- Liu, J., Luo, C., Lu, H., Huang, Z., Long, G., dan Peng, X., 2022, Influence of Hexagonal Boron Nitride on Electronic Structure of Graphene, *Molecules*, Vol. 27, no. 12
- Perdew, J. P., Burke, K., dan Ernzerhof, M., 1996, Generalized Gradient Approximation Made Simple, *Physical Review Letters*, Vol. 77, no. 18, pp 3865–3868
- Perdew, J. P. dan Zunger, A., 1981, Self-interaction correction to density-functional approximations for many-electron systems, *Physical Review B*, Vol. 23, no. 10, pp 5048–5079
- Phung, V. B. T., Pham, B. L., Duy, N. V. A., Dang, M. T., Tran, T. N., Tran, Q. H., Luong, T. T., dan Dinh, V. A., 2024, First-principles study of highly sensitive graphene/hexagonal boron nitride heterostructures for application in toxic gas-sensing devices, *RSC Advances*, Vol. 14, no. 7, pp 4904–4916
- Podaru, N., 2011, Tailoring the electronic structure properties of carbon based materials, *Atmospheric Environment - ATMOS ENVIRON*, Advance Access published 1 Januari 2011
- Salvatella, L., 2025, Rethinking Organic Chemistry: The Dual Electronic Behavior of the Alkyl Group, *Journal of Chemical Education*, Vol. 102, no. 11, pp 4666–4675
- Sani, H., Kubota, T., dan Surahman, U., 2023, Factors affecting multiple chemical sensitivity (MCS) in newly constructed apartments of Indonesia, *Building and Environment*, Vol. 241
- Siahaan, P., Wafiyah, S., Abid, M. B., Hudiyanti, D., Hildayani, S. Z., Windarti, T., Asy'ari, M., dan Sakti, A. W., 2026, Structural, Electronic, and Optical Properties of Bi-Doped Cubic Lead-Free Perovskite CsSnBr₃: A Density Functional Theory Study, *Journal of Inorganic and Organometallic Polymers and Materials*, Advance Access published 15 Mei 2026: doi:10.1007/s10904-026-04341-6
- Szyniszewski, M., Mostaani, E., Knothe, A., Enaldiev, V., Ferrari, A. C., Fal'ko, V. I., dan Drummond, N. D., 2025, Adhesion and Reconstruction of Graphene/Hexagonal Boron Nitride Heterostructures: A Quantum Monte Carlo Study, *ACS Nano*, Vol. 19, no. 6, pp 6014–6020

- Tian, Q., 2019, *Introduction to adsorption : basics, analysis, and applications*, Elsevier, Amsterdam, Netherlands
- Tuan Hung, N., Nugraha, A. R. T., dan Saito, R., 2022, *Quantum ESPRESSO Course for Solid-State Physics*, Jenny Stanford Publishing
- Ullah, N., Zhang, R. Q., Murtaza, G., Yar, A., dan Mahmood, A., 2016, Stacking nature and band gap opening of graphene: Perspective for optoelectronic applications, *Solid State Communications*, Vol. 246, pp 54–58
- Vázquez-Parga, D., Fernández-Martínez, A., dan Viñes, F., 2023, Quantifying the Accuracy of Density Functionals on Transition Metal Bulk and Surface Properties, *Journal of Chemical Theory and Computation*, Vol. 19, no. 22, pp 8285–8292
- Vera, S. M., Mennickent, S. C., Gómez-Gaete, C., dan Rogel, C. C., 2024, Health risk due to the chronic use of formaldehyde in workplace settings and as a component of hair straightening products; [Riesgos en la salud del uso crónico de formaldehído en el ámbito laboral y como componente de productos de alisado capilar], *Horizonte Medico*, Vol. 24, no. 2
- Wang, J., Ma, F., dan Sun, M., 2017, Graphene, hexagonal boron nitride, and their heterostructures: properties and applications, *RSC Advances*, Vol. 7, no. 27, pp 16801–16822
- Wang, Q. dan Xiao, K., 2022, Indoor Formaldehyde Concentrations and the Influencing Factors in Urban China, *Progress in Chemistry*, Vol. 34, no. 3, pp 743–772
- Xu, B., Lv, M., Fan, X., Zhang, W., Xu, Y., dan Zhai, T., 2015, Lattice Parameters of Hexagonal and Cubic Boron Nitrides at High Temperature and High Pressure, *Integrated Ferroelectrics*, Vol. 162, pp 85–93
- Zhang, L., Wang, B., Li, K., Wang, Z., Xu, D., Su, Y., Wu, D., dan Xie, B., 2023, Non-negligible health risks caused by inhalation exposure to aldehydes and ketones during food waste treatments in megacity Shanghai, *Environmental Pollution*, Vol. 325