



## DAFTAR PUSTAKA

- Afreen, S., Muthoosamy, K., Manickam, S., & Hashim, U. (2015). Functionalized fullerene (C<sub>60</sub>) as a potential nanomediator in the fabrication of highly sensitive biosensors. *Biosensors and Bioelectronics*, 63, 354–364. <https://doi.org/10.1016/j.bios.2014.07.044>
- Aly, F. M., Othman, A., & Hardiy, M. (2018). Protective Effects of Fullerene C<sub>60</sub> Nanoparticles and Virgin Olive Oil against Genotoxicity Induced by Cyclophosphamide in Rats. *Oxidative Medicine and Cellular Longevity*, 1–12. <https://doi.org/10.1155/2018/1261356>
- Alyar, S., Sen, T. A., Özmen, Ü. Ö., Alyar, H., Adem, S., & Sen, C. (2019). Synthesis, spectroscopic characterizations, enzyme inhibition, molecular docking study and DFT calculations of new Schiff bases of sulfa drugs. *Journal of Molecular Structure*, 1185, 416–424. <https://doi.org/10.1016/j.molstruc.2019.03.002>
- Bashiri, S., Vessally, E., Bekhradnia, A., Hosseinian, A., Edjlali, L. (2017). Utility of extrinsic [60] fullerenes as work function type sensors for amphetamine drug detection: DFT studies, *Vacuum*, 136, 156162.
- Beaser, A. (1992). Konsep Fisika Modern. Eriangga, Jakarta.
- Billas, I. M. L., Massobrio, C., Boero, M., Parrinello, M., Branz, W., Tast, F., Malinowski, N., Heinebrodt, M., & Martin, T. (1999). First principles calculations of Si doped fullerenes: Structural and electronic localization properties in C<sub>59</sub>Si and C<sub>58</sub>Si<sub>2</sub>. *Journal of Chemical Physics*, 111(15), 6787–6796. <https://doi.org/10.1063/1.480018>
- Born, M., Oppenheimer, R. (1927). Zur Quantentheorie der Moleküle. *Ann. Phys*, 389, 457.
- Bouachrine, Si Mohamed. (2011). OLIGOTHIOPHENES BRIDGED BY SILICON GROUPS, DFT STUDY OF STRUCTURAL AND ELECTRONIC PROPERTIES.. *Phys. Chem. News* 58 (2011) 61-66. 58. 61.



- Burke, K., dan Wagner, L. O. (2013): *DFT in a nutshell*, International Journal of Quantum Chemistry. 113, 96-101
- Cedervall, T., Lynch, I., Lindman, S., Berggård, T., Thulin, E., Nilsson, H., Dawson, K. A., & Linse, S. (2007). Understanding the nanoparticle–protein corona using methods to quantify exchange rates and affinities of proteins for nanoparticles. *Proceedings of the National Academy of Sciences of the United States of America*, 104(7), 2050–2055. <https://doi.org/10.1073/pnas.0608582104>
- Chaudhary, M. K., Srivastava, A., Singh, K. K., Tandon, P., & Joshi, B. D. (2020). Computational evaluation on molecular stability, reactivity, and drug potential of frovatriptan from DFT and molecular docking approach. *Computational and Theoretical Chemistry*, 1191, 113031. <https://doi.org/10.1016/j.comptc.2020.113031>
- Cioslowski, J. (1991) Endohedral Chemistry: Electronic Structures of Molecules Trapped inside the C<sub>60</sub> Cage. *Journal of the American Chemical Society*, 113, 4139-4141. <http://dx.doi.org/10.1021/ja00011a013>
- Conde, J. et al. (2011) Nanophotonics for molecular diagnostics and therapy applications, *International Journal of Photoenergy*. Hindawi. Available at: <https://www.hindawi.com/journals/ijp/2012/619530/> (Accessed: April 6, 2023).
- B. Ramachandran, *Structure, stability, and properties of boron encapsulated complexes of C<sub>60</sub>, C<sub>59</sub>B, dan C<sub>59</sub>N*, *J. Phys. Chem. A* 121 (2017) 1708.
- Calabresi P, Picconi B, Tozzi A, Di Fillippo M. *Dopamine-mediated regulation of corticostriatal synaptic plasticity*. Trends in Neurosciences. 2007;30(5):211219
- Das, P. K., Bakuli, S., Samanta, A., Mandal, A. K., Ghosh, J., Dey, A., & Mukhopadhyay, A. K. (2017). Very high Cu(II) adsorption efficacy of designed nano-platelet Mg(OH)<sub>2</sub> assembly. *Materials Research Express*, 4(2), 025025. <https://doi.org/10.1088/2053-1591/aa5cd1>
- Echt, O., Kaiser, A., Zottl, S., Mauracher, A., Denifl, S., Scheier, P., 2013, *Adsorption of Polar and Nonpolar Molecules on Isolated Cationic C<sub>60</sub>, C<sub>70</sub>, and Their Aggregates*, *ChemPlusChem* 78, 910-920.



- Esrafili, M. D., & Janebi, H. (2020). B-, N-doped and BN codoped C<sub>60</sub> heterofullerenes for environmental monitoring of NO and NO<sub>2</sub>: a DFT study. *Molecular Physics*, 118(5). <https://doi.org/10.1080/00268976.2019.1631495>
- Ferenczy, G. G., Harsányi, L., Rozsondai, B., & Hargittai, I. (1986). The molecular structure of uracil: an electron diffraction study. *Journal of Molecular Structure*, 140(1–2), 71–77. [https://doi.org/10.1016/0022-2860\(86\)80148-x](https://doi.org/10.1016/0022-2860(86)80148-x)
- Fowler, J.D., Allen, M.J., Tung, V.C., Yang, Y., Kaner, R.B., Weiler, B.H. (2009) *Practical Chemical Sensors from Chemically Derived Graphene*, ACS Nano, 301-306.
- Gao, X., Kim, K., & Liu, D. (2007). Nonviral gene delivery: What we know and what is next. *Aaps Journal*, 9(1), E92–E104. <https://doi.org/10.1208/aapsj0901009>
- Gatica, S. M., Nekhai, A., & Scrivener, A. (2016). Adsorption and Gas Separation of Molecules by Carbon Nanohorns. *Molecules*, 21(5), 662. <https://doi.org/10.3390/molecules21050662>
- Gehrke, T., & Zeeb, B. P. (2019). Uracil in RNA: versatile and multifunctional. *Accounts of Chemical Research*, 52(11), 3124-3136.
- Georgakilas, V., Pellarini, F., Prato, M., Guldi, D.M., Melle-Franco, M., Zerbetto, F., (2002). *Supramolecular Self-Assembled Fullerene Nanostructures*, PNAS 99, 5075-5080.
- Gillespie, R. J. (2004). Teaching Molecular Geometry with the VSEPR Model. *Journal of Chemical Education*, 81(3), 298. <https://doi.org/10.1021/ed081p298>
- Gokpek, Y., Bilge, M., Bilge, D., Alver, Ö., & Parlak, C. (2017). Adsorption mechanism, structural and electronic properties: 4-Phenylpyridine & undoped or doped (B or Si) C<sub>60</sub>. *Journal of Molecular Liquids*, 238, 225–228. <https://doi.org/10.1016/j.molliq.2017.04.128>
- Griffiths, D. J. (1994): *Introduction to Quantum Mechanics*: Englewood Cliffs, NJ Prentice-Hall.



- Gross, E. K. U., & Kohn, W. (1990). Time-Dependent Density-Functional Theory. *Advances in Quantum Chemistry*, 255–291. [https://doi.org/10.1016/s0065-3276\(08\)60600-0](https://doi.org/10.1016/s0065-3276(08)60600-0)
- 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, 89.
- Hassani, F., Tavakol, H., 2014, *A DFT, AIM and NBO study of adsorption and chemical sensing of iodine by S-doped fullerenes*, *Sensors and Actuators B: Chemical*, 196, 624630.
- Hazrati, M.K., Hadipour, N.L., 2016, Adsorption behavior of 5-fluorouracil on pristine, B-,Si-, and Al-doped C60 fullerenes : A first-principle study, *Physics Letters A* 380, 937-941.
- Hohenberg, P., and Kohn, W., 1964, Phys. Rev. B 136, 864.
- Hohenberg, P., and Kohn, W., 1964, Inhomogeneous Electron Gas, Physical Review B, Vol.136
- Hu, X., Ren, G., Xu, Y., Zhu, Z., Liu, J., Ma, X., ... & Wang, J. (2020). Structural and thermodynamic studies of nucleic acid base pairs. International journal of molecular sciences, 21(10), 3524.
- Igumbor, E. (2017): *Hybrid functional study of point defects in germanium*. Tesis, Fakultas Ilmu Pengetahuan Alam dan Pertanian, Universitas Pretoria.
- J. Kaur, G.S. Gill, K. Jeet, in: *Application of carbon nanotubes in drug delivery: A comprehensive review*, 2019, p. 113.
- J. Shi, B. Wang, L. Wang, T. Lu, Y. Fu, H. Zhang, Z. Zhang, *Fullerene (C<sub>60</sub>)-based tumor-targeting nanoparticles with “off-on” state for enhanced treatment of cancer*, J. Control. Release 235 (2016) 245–258.
- Jana, S., Chodvadiya, D., Som, N. N., & Jha, P. K. (2022). A quantum mechanical prediction of C24 fullerene as a DNA nucleobase biosensor. *Diamond and Related Materials*, 129, 109305.



- JMOL, <http://jmol.sourceforge.net/>.
- JMOL-MEP, <https://www.cup.uni-muenchen.de/ch/compchem/pop/mep>
- Kaviani, B. (2015). Theoretical Investigation of Luminescent Defects in Diamond. Universitaatsbibliothek Bremen, <https://elib.suub.unibremen.de/edocs/00104254-1.pdf>
- Kim, C., & Kymmissis, I. (2017). Graphene–organic hybrid electronics. *Journal of Materials Chemistry C*, 5(19), 4598–4613. <https://doi.org/10.1039/c7tc00664k>
- Kohanoff, J., Gidopoulos, N.I. (2003). Density Functional Theory: Basics, New Trends and Applications, Handbook of Molecular Physics and Quantum Chemistry, Vol.2, Part 5, Chapter 26, 532-568, John Wiley and Sons, Ltd, Chichester
- Kohn, W. (1999). Electronic structure of matter-wave functions and density functionals, Department of Physics, University of California, Santa Barbara, Nobel Lecture.
- Kohn, W., dan Sham, L. (1965): Self-Consistent Equations Including Exchange and Correlation Effects, *Physical Review*, 140, 33-38.
- Krätschmer, W., Lamb, L. D., Fostiropoulos, K., & Huffman, D. R. (1990). Solid C<sub>60</sub>: a new form of carbon. *Nature*, 347(6291), 354–358. <https://doi.org/10.1038/347354a0>
- Kroto, H., Heath, J., Obrien, S. et al, (1985). C<sub>60</sub>: Buckminsterfullerene. *Nature* 318, 162163.
- Kweitsu, E. K., Armoo, S. K., Kan-Dapaah, K., Abavare, E. K. K., Dodoo-Arhin, D., & Yaya, A. (2020). Comparative Study of Phosgene Gas Sensing Using Carbon and Boron Nitride Nanomaterials—A DFT Approach. *Molecules*, 26(1), 120. <https://doi.org/10.3390/molecules26010120>
- Lewinski, N., Colvin, V. L., & Drezek, R. A. (2008). Cytotoxicity of Nanoparticles. *Small*, 4(1), 26–49. <https://doi.org/10.1002/smll.200700595>
- Lipkowski, P., Kozlowska, J., & Bartkowiak, W. (2021). A Look at the Spatial Confining Effect on the Molecular Electrostatic Potential (MEP)—A Case Study



- of the HF and BrCN Molecules. *Molecules*, 26(19), 5924. <https://doi.org/10.3390/molecules26195924>
- Liu, J.H., Cao, L., Luo, P.G., Yang, S.T., Lu, F., Wang, H., Meziani, M.J., Haque, S.A., Liu, Y., Lacher, S., Sun, Y.P. (2010). Fullerene-Conjugated doxorubicin in cells, *ACS Appl. Mater Interfaces*, 13847-9.
- Kumar, K. Raza, *C<sub>60</sub>-Fullerene as drug delivery carriers for anticancer agents: promises and hurdles*, *Pharm. Nanotechnol.* 5 (2017) 169.
- Maeta, T., dan Sueoka, K. (2014). Density functional theory calculations of stability and diffusion mechanisms of impurity atoms in Ge crystals, *Journal of Applied Physics*, 116(7), 073505.
- Maleki, R., Khoshoei, A., Rashidi, A., & Rashidi, A. (2020). Molecular insight into the smart functionalized TMC-Fullerene nanocarrier in the pH-responsive adsorption and release of anti-cancer drugs. *J Mol Graph Model*, 100, 107660. <https://doi.org/10.1016/j.jmgm.2020.107660>
- Marks, L. D. (2021). Predictive Mixing for Density Functional Theory (and Other Fixed-Point Problems). *Journal of Chemical Theory and Computation*, 17(9), 5715–5732. <https://doi.org/10.1021/acs.jctc.1c00630>
- Marsusi, F., & Qasemnazhand, M. (2016). Sila-fulleranes: promising chemically active fullerene analogs. *Nanotechnology*, 27(27), 275704. <https://doi.org/10.1088/0957-4484/27/27/275704>
- Martínez, A. (2021). Electron donor–acceptor capacity of selected pharmaceuticals against COVID-19. *Antioxidants*, 10(6), 979. <https://doi.org/10.3390/antiox10060979>
- Medrek, M., Plucinski, F., Mazurek, A.P. (2013). Endohedral Complexes of Fullerene C<sub>60</sub> with small covalent molecules (H<sub>2</sub>O, NH<sub>3</sub>, H<sub>2</sub>, 2H<sub>2</sub>, 3H<sub>2</sub>, 4H<sub>2</sub>, O<sub>2</sub>, O<sub>3</sub>) in the context of potential drug transport system, *Acta Poloniae Pharmaceutica Drug Research*, 70-4, 659-665.



- Mohammadi, M., & Abdullah, H. Y. (2021). Non-covalent interactions of cysteine onto C<sub>60</sub>, C<sub>59</sub>Si, and C<sub>59</sub>Ge: a DFT study. *Journal of Molecular Modeling*, 27(11). <https://doi.org/10.1007/s00894-021-04960-5>
- Montellano, A., Da Ros, T., Bianco, A., & Prato, M. (2011). Fullerene C<sub>60</sub> as a multifunctional system for drug and gene delivery. *Nanoscale*, 3(10), 4035. <https://doi.org/10.1039/c1nr10783f>
- Moradi, M., Nouraliei, M., Moradi, R. (2017). Theoretical study on the phenylpropanolamine drug interaction with the pristine, Si and Al doped [60] fullerenes, *Physica E*, 87, 186191.
- NA Standards | Valence Geometries | Bond Lengths & Angles - Uracil. (n.d.). <http://ndbserver.rutgers.edu/ndbmodule/archives/proj/valence/bases5.html>
- Njeumen, C. A., Ejuh, G. W., Assatse, Y. T., Kamsi, R. a. Y., & Ndjaka, J. M. B. (2023). DFT studies of physico-chemical, electronic and nonlinear optical properties of interaction between doped-fullerenes with non-steroidal anti-inflammatory drugs. *Physica B-condensed Matter*, 665, 415041. <https://doi.org/10.1016/j.physb.2023.415041>
- Ö. Alver, C. Parlak, M. Şenyel. (2007). and nJCH coupling constants investigation of 4-phenylpyridine: a combined experimental and theoretical study, *Phys. Lett. A* 371 300–306.
- OVPN, <http://ovpn.com/en>.
- Oswald, J., Beretta, D., Stiefel, M., Furrer, R., Vuillaume, D., & Calame, M. (2023). The Effect of C<sub>60</sub> and Pentacene Adsorbates on the Electrical Properties of CVD Graphene on SiO<sub>2</sub>. *Nanomaterials*, 13(6), 1134. <https://doi.org/10.3390/nano13061134>
- Park, S. K., Jeong, J., Rha, S., Park, S. W., Cho, M. H., Cho, S. H., Yi, Y., Heo, M., & Sohn, H. (2010). The electronic structure of C<sub>60</sub>/ZnPc interface for organic photovoltaic device with blended layer architecture. *Applied Physics Letters*, 96(1). <https://doi.org/10.1063/1.3285174>



- Parlak, C., Alver, O. (2017). A density functional theory investigation on amantadine drug interaction with pristine and B, Al, Si, Ga, Ge doped C<sub>60</sub> fullerenes, *Chem. Phys. Lett.*, 678, 8590.
- Parr, R. G., dan Weitao, Y. (2015): Density-Functional Theory of Atoms and Molecules, Oxford University,  
<http://public.eblib.com/choice/publicfullrecord.aspx?p=4702301>.
- Perdew, J.P., Burke, K., Ernzerhof, M. (1996). Generalized Gradient Approximation Made Simple, *Phys. Rev.*, 77, 18.
- Perdew, J. P., Chevary, J. A., Vosko, S. H., Jackson, K. A., Pederson, M. R., Singh, D. J., dan Fiolhais, C. (1992): Atoms, molecules, solids, and surfaces: Applications of the generalized gradient approximation for exchange and correlation, *Physical Review B*. 46, 6671-6687.
- Pérez-Ruiz, J. M., Santos-Pérez, L. A., & Becerra-Flores, M. (2021). Uracil and the Central Dogma of Molecular Biology. In Biochemistry and Molecular Biology: Concepts, Methodologies, Tools, and Applications (pp. 282-301). IGI Global.
- PHASE, <http://azuma.nims.go.jp>.
- Prato, M. (1997). [60]Fullerene chemistry for materials science applications. *Journal of Materials Chemistry*, 7(7), 1097–1109. <https://doi.org/10.1039/a700080d>
- PubChem. (n.d.). <https://pubchem.ncbi.nlm.nih.gov/>
- Rabenau, T., Simon, A. R., Kremer, R. K., & Sohmen, E. (1993). The energy gaps of fullerene C<sub>60</sub> and C<sub>70</sub> determined from the temperature dependent microwave conductivity. *Zeitschrift Für Physik*, 90(1), 69–72.  
<https://doi.org/10.1007/bf01321034>
- Rad, A. S., Aghaei, S. M., Aali, E., Peyravi, M., & Jahanshahi, M. (2018). Application of chromium-doped fullerene as a carrier for thymine and uracil nucleotides: Comprehensive density functional theory calculations. *Applied Organometallic Chemistry*, 32(2). <https://doi.org/10.1002/aoc.4070>
- Raphey V, Henna T, Nivitha K, Mufeedha P, Sabu C, Pramod K. (2019). Biomedical



- applications from carbon nanotube applications. *Mater Sains Ind, C* 100: 616–630. <https://doi.org/10.1016/j.mdtk.2019.03.043> 1951.
- Shahnazari, G. H., & Ganji, M. D. (2021b). Understanding structural and molecular properties of complexes of nucleobases and Au<sub>13</sub> golden nanocluster by DFT calculations and DFT-MD simulation. *Scientific Reports*, 11(1). <https://doi.org/10.1038/s41598-020-80161-z>
- Sholihun, (2015). First-Principles Calculations of Vacancies in Semiconductors, thesis University of Kanazawa, Japan.
- Silva, R. O. S., Machado, D. A., De Oliveira, H. C. B., Ribeiro, L., & Da Silva Filho, D. A. (2022b). Theoretical study of the interaction of fullerenes with the emerging contaminant carbamazepine for detection in aqueous environments. *Scientific Reports*, 12(1). <https://doi.org/10.1038/s41598-022-19258-6>
- Slater, J.C. (1951): A simplification of the Hartree-Fock method, *Physical Review*, 81 (3), p.385.
- Umam K, Sholihun, Nurwantoro P, Nugraheni A.D, Budhi R.H.S. (2018). *J. Phys. Conf. Ser.* 1011(1) 012074.
- VESTA, <https://jp-minerals.org/vesta/en/>.
- Wang, P., Yan, G., Zhu, X., du, Y., Chen, D., Zhang, J. (2021). *Heterofullerene MC59 (M = B, Si, Al) as Potential Carriers for Hydroxyurea Drug Delivery*, *Nanomaterials* 11, 115.
- Wang, Y., Zhang, H., & Huang, L. (2015). Smart Polymeric Nanoparticles for Cancer Gene Delivery. *Molecular Pharmaceutics*, 12(2), 314–321. <https://doi.org/10.1021/mp500656v>
- WinSCP, <https://winscp.net/eng/download.php>.
- X. Sun, Z. Liu, K. Welsher, J.T. Robinson, A. Goodwin, S. Zaric, H. Dai. (2008). *Nanographene oxide for cellular imaging and drug delivery*, *Nano Res.* 1 203.
- Xie, J., Wang, L., Wu, X., Huang, X., Liu, Y., Chen, X., ... & Zhang, H. (2020). Chemical modifications of adenine and guanine residues in DNA: biological significance. *Chemical Society Reviews*, 49(20), 7335-7363.



Yousefian, Z., Rashidi, A., & Kooti, M. (2019). Theoretical studies on B, N, P, S, and Si doped fullerenes toward H<sub>2</sub>S sensing and adsorption. *Physica E-Low-Dimensional Systems & Nanostructures*, 114, 113626.  
<https://doi.org/10.1016/j.physe.2019.113626>

Zhang, D., Lu, C., & Wu, W. (2020). A thymine derivative-induced DNA hydrogel for detection of DNA damage. *Chemical Communications*, 56(85), 13166-131