



DAFTAR PUSTAKA

- Afreen, S., Muthoosamy, K., Manickam, S., Hashim, U., 2014, Functionalized Fullerene (C_{60}) as a potential nanomediator in the fabrication of highly sensitive biosensors, *Biosens Bioelectron* 63, 354-364.
- ASHP (American Society of Health-System Pharmacists)., 2021, <https://www.drugs.com/monograph/hydroxyurea.html> diakses Agustus 2021.
- 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.
- Born, M., Oppenheimer, R., 1927, Zur Quantentheorie der Moleküle. *Ann. Phys.*, 389, 457.
- Cioslowski, J., 1991, Endohedral Chemistry : Electronic Structure of Molecules Trapped Inside the C_{60} Cage, *J.Am.Chem.Soc* 113, 4139-4141.
- Echt, O., Kaiser, A., Zöttl, S., Mauracher, A., Denifl, S., Scheier, P., 2013, Adsorption of Polar and Nonpolar Molecules on Isolated Cationic C_{60} , C_{70} , and Their Aggregates, *ChemPlusChem* 78, 910-920.
- Esrafili, M.D., Janebi, H., 2020, B-, N- doped dan BN codoped C_{60} heterofullerenes for environmental monitoring of NO and NO_2 : a DFT study, *Molecular Physics*, 118:5.
- 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.
- Gatica, S.M., Nekhai, A., dan Scrivener, A., 2016, Adsorption and Gas Separation by Carbon Nanohorns, *Molecules* 21, 662.



Georgakilas, V., Pellarini, F., Prato, M., Guldin, D.M., Melle-Franco, M., Zerbetto, F., 2002, Supramolecular Self-Assembled Fullerene Nanostructures, *PNAS* 99, 5075-5080.

Gokpek, Y., Bilge, M., Bilge, D., Alver, O., Parlak, C., 2017, Adsorption mechanism, structural and electronic properties: 4-Phenylpyridine and undoped or doped (B or Si) C₆₀, *J. Mol. Liq.*, 238, 225228.

Hartree, D.R., 1928, Proc. Cambridge, *Phil. Soc.* 24:89, 426.

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

JMOL, <http://jmol.sourceforge.net/>.

JMOL-MEP, <https://www.cup.uni-muenchen.de/ch/compchem/pop/mep1.html>.

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., and Sham, L.J., 1965, Self-Consistent Equations Including Exchange and Correlations Effects, *Physical Review A*, Vol.140.

Kroto, H., Heath, J., O'Brien, S. et al, 1985, C₆₀: Buckminsterfullerene. *Nature* 318, 162163.



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.

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.

Medrek, M., Plucinski, F., Mazurek, A.P, 2013, Endohedral Complexes of Fullerene C_{60} with small covalent molecules (H_2O , NH_3 , H_2 , $2H_2$, $3H_2$, $4H_2$, O_2 , O_3) in the context of potential drug transport system, *Acta Poloniae Pharmaceutica-Drug Research*, 70-4, 659-665.

Mohammadi, M.R., Nojoomi, A., Mozafari, M., Dubnika, A., Inayathullah, M., Rajadas, J, 2017, Nanomaterials engineering for drug delivery : a hybridization approach, *J. Mater. Chem. B*.

Montellano, A., Ros, T.D., Bianco, A., Prato, M, 2011, Fullerene C_{60} as multifunctional system for drug and gene delivery, *Nanoscale* 3, 4035.

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.

Novir, S.B., Aram, M.R, 2020, Quantum mechanical simulation of Chloroquine drug interaction with C60 fullerene for treatment of COVID-19, *Chemical Physics Letters*, 757, 137869.

OVPN, <http://ovpn.com/en>.

Parlak, C., Alver, O, 2017, A density functional theory investigation on amantadine drug interaction with pristine and B, Al, Si, Ga, Ge doped C60 fullerenes, *Chem. Phys. Lett*, 678, 8590.



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., 1992, Atoms, Molecules, Solids, and Surfaces: Applications of the Generalized Gradient Approximation for Exchange and Correlation, *Phys. Rev. B*, 48, 11.

PHASE, <http://azuma.nims.go.jp>.

Prato, M., 1997, [60]Fullerene chemistry for materials science applications, *J. Mater. Chem* 7(7), 1097-1109.

Sholihun., 2015, Thesis: *First-Principles Calculations of Vacancies in Semiconductors*, University of Kanazawa, Japan, hal 1-6 dan 7-30.

Stewart, Judith., 2021, <https://www.drugs.com/paracetamol.html> diakses Agustus 2021.

VESTA, <https://jp-minerals.org/vesta/en/>.

Wang, P., Yan, G., Zhu, X., du, Y., Chen, D., Zhang, J., 2021, Heterofullerence MC_{59} (M = B, Si, Al) as Potential Carriers for Hydroxyurea Drug Delivery, *Nanomaterials* 11, 115.

WinSCP, <https://winscp.net/eng/download.php>.

Zakharian, T.Y., Seryshev, A., Sitharman, B., Gilbert, B.G., Knight, V., Wilson, L.J., 2005, A Fullerene-Paclitaxel Chemotherapeutic : Synthesis, Characterization, and Study of Biological Activity in Tissue Culture, *J. Am. Chem. Soc* 127-36, 12508-12509.