

REFERENCES

- Ammar, A.M., Mohamed, H.S.H., Yousef, M.M.K., Abdel-Hafez, G.M., Hassanien, A.S., and Khalil, A.S.G., 2019, Dye-Sensitized Solar Cells (DSSCs) based on extracted natural dyes, *J. Nanomater.*, 2019, 1-10.
- Anastas, P.T., 2007, Introduction: Green Chemistry, *Chem. Rev.*, 107 (6), 2167-2168;
- Atkins, P.W. and de Paula, J., 2006, *Physical Chemistry*, Oxford University Press, Oxford.
- Aziz, H.A., 2015, Kajian Pengaruh Substituen Terhadap Sifat Kompleks Semikonduktor Hg(II)-Porfirin dengan Metode Density Functional Theory/Time Dependent-Density Functional Theory (DFT/TD-DFT), *Skripsi*, Departemen Kimia FMIPA UGM, Yogyakarta.
- Baker, J., Scheiner, A., and Andzelm, J., 1993, Spin Contamination in Density Functional Theory, *Chem. Phys. Lett.*, 216 (3), 380-388.
- Barbee, J. and Kuznetsov, A.E., 2011, Revealing Substituent Effects on the Electronic Structure and Planarity of Ni(II)-porphyrins, *Comput. Theo. Chem.*, 981,73-85.
- Becke, A.D., 1992, A New Mixing of Hartree-Fock and Local Density-Functional Theories, *Chem. Phys.*, 98, 1372-1377.
- Beni, S.A., Zarandi, M., Hosseinzadeh, B., and Chermahini, N.A., 2018, Density Functional Theory Study of Carbazole Dyes: Potential Application of Carbazole Dyes in Dye-Sensitized Solar Cells, *J. Mol. Struct.*, 1164, 155–163.
- Biswas, S., 2013, Optimization of Nanowire Photodiode Devices for Neuronal Cell Survival, *Thesis*, Department of Physics of Lund University, Sweden.
- Bruss, L.E., 1984, Electron-Electron and Electron Hole Interactions in Small Semiconductor Crystallites: The Size Dependence of the Lowest Excited Electronic State, *J. Chem. Phys.*, 80(9), 4403-4409.
- Busch, G., 1989, Early History of the Physics and Chemistry of Semiconductors—from Doubts to Fact in a Hundred Years, *Eur. J. Phys.*, 10, 254–264.
- Collins, T.J., 1995, Introducing Green Chemistry in Teaching and Research, *J. Chem. Educ.*, 72, 965–966.
- Cook, L., Brewer, G., and Wong-Ng, W., 2017, Structural Aspects of Porphyrins for Functional Materials Application, *Crystals*, 7(7), 223.
- Ditchfield, R., Hehre, W.J., and Pople J.A., 1971, Self-Consistent Molecular Orbital Method IX. An Extended Gaussian Type Basis for Molecular-Orbital Studies of Organic Compounds, *J. Chem. Phys.*, 54, 724-729.

- Dy, E.S. and Kasai, H., 2005, Characterization of Platinum Porphyrins and its Interaction with Oxygen by Density Functional Theory, *e-Journal Surf. Sci. Nanotechnol.*, 3, 473–475.
- Facchetti, A., 2011, π -Conjugated Polymers for Organic Electronics and Photovoltaic Cell Applications, *Chem. Mater.*, 23, 733–758.
- Fichou, D. and Horowitz, G., 2001, Molecular and Polymer Semiconductors, Conductors, and Superconductors: Overview, *Encycl. Mater. Sci. Technol.*, 5748–5757.
- Güngör, S.A., Köse, M., Tümer, F., and Tümer, M., 2016, Photoluminescence, Electrochemical, SOD Activity and Selective Chemosensor Properties of Novel Asymmetric Porphyrin-Schiff Base Compounds, *Dyes Pigm.*, 130, 37–53.
- Hehre, W.J., Stewart, R.F., and Pople, J.A., 1969, Self-Consistent Molecular-Orbital Method I. Use of Gaussian Expansion of Slater Type Atomic Orbitals, *J. Chem. Phys.*, 51, 2657-2665.
- Hjeresen, D.L., Boese, J.M., and Schutt, D.L., 2000, Green Chemistry and Education, *J. Chem. Educ.*, 77 (12), 1543.
- Hodes, G., 2011, *Electrochemistry of Nanomaterials*, Wiley-VCH, Weinheim.
- Juma, J.M., Vuai, S.A.H., and Surendra Babu, N., 2019, TD-DFT investigations on Optoelectronic Properties of Fluorescein Dye Derivatives in Dye-Sensitized Solar Cells (DSSCs), *Int. J. Photoenergy*, 2019(9),1-8.
- Juster, N.J., 1963, California Association of Chemistry Teachers, *J. Chem. Educ.*, 40, 547–555.
- Keyman, 2019, Kajian Teoritik Pengaruh Jumlah dan Posisi Substituen Terhadap Struktur dan Sifat Semikonduktor Kompleks Logam Alkali Tanah (Be, Mg, dan Ca) Porfirin dengan Metode Teori Fungsional Kerapatan, *Skripsi*, Departemen Kimia FMIPA UGM, Yogyakarta.
- Kohn, W. and Sham, L.J., 1965, Self Consistent Equation Including Exchange and Correlation Effects, *Phys. Rev.*, 140, A1133-A1138.
- Krishnan, R., Binkley, J.S., Seeger, R., and Pople, J.A., 1980, Self-Consistent Molecular-Orbital Method XX. A Basis Set for Correlated Wave Function, *J. Chem. Phys.*, 72, 650-654.
- Kruse, H., Goerigk, L., and Grimme, S., 2012, Why the Standard B3LYP/6-31* Model Chemistry Should Not Be Used in DFT Calculation of Molecular Thermochemistry: Understanding and Correcting the Problem, *J. Org. Chem.*, 77 (23), 10824-10834.
- Lee, C., Yang, W., and Parr, R.G., 1988, Development of Colle-Salvetti correlation Energy Formula into a Functional of the Electron Density, *Phys. Rev. B.*, 37, 785-789.

- McCreery, R.L., 2004, Molecular Electronic Junctions, *Chem. Mater.*, 16, 4477–4496.
- Milot, R.L. and Schmuttenmaer, C.A., 2015, Electron Injection Dynamics in High-Potential Porphyrin Photoanodes, *Acc. Chem. Res.*, 48(15), 1423-1431.
- Mink, L.M., Neitzel, M.L., Bellomy, L.M., Falvo, R.E., Boggess, R.K., Trainum, B.T., and Yeaman, P., 1997, Platinum(II) and Platinum(IV) Porphyrin Complexes: Synthesis, Characterization, and Electrochemistry, *Polyhedron*, 16(16), 2809–2817.
- Monti, O.L.A., 2012, Understanding Interfacial Electronic Structure and Charge Transfer: An Electrostatic Perspective, *J. Phys. Chem. Lett.*, 3, 2342–2351.
- Mulya, F., 2015, Kajian Pengaruh Substituent Terhadap Sifat Semikonduktor Platina(II) Porfirin dengan Metode Density Functional Theory (DFT), *Skripsi*, Departemen Kimia FMIPA UGM, Yogyakarta.
- Mulya, F., Santoso, G.A., Aziz, H.A., and Pranowo, H.D., 2016, Design a Better Metalloporphyrin Semiconductor: A Theoretical Studies on the Effect of Substitents and Central Ions, *AIP Conf. Proc.*, 1755, 080006.
- O'Boyle, N.M., Tenderholt, A.L., and Lagner, K.M., 2008, CCLIB: A Library For Package Independent Computational Chemistry Algorithm, *J. Comput. Chem.*, 29 (5), 839-845.
- Ogumi, K., Nakagawa, T., Okada, H., and Matsuo, Y., 2019, Improved Solubility of Asymmetric Tetraethynylporphyrin Derivatives for Solution-Processed Organic Solar Cells, *Org. Electron.*, 71, 50–57.
- Pranowo, H.D., Mulya, F., Aziz, H.A., and Santoso, G.A., 2018, Study of Substituent Effect on Properties of Platinum(II) Porphyrin Semiconductor Using Density Functional Theory, *Indones. J. Chem.*, 18, 742-748.
- Sánchez-Bojorge, N.A., Zaragoza-Galán, G., Flores-Holguín, N.R., Chávez-Rojo, M.A., Castro-García, C., and Rodríguez-Valdez, L.M., 2019, Theoretical Analysis of the Electronic Properties in Zinc-Porphyrins Derivatives, *J. Mol. Struct.*, 1191, 259–270.
- Shalabi, A.S., Assem, M.A., Soliman, K.A., El Mahdy, A.M., and Taha, H.O., 2014, Performance of Metalloporphyrin Malonic Acid as Dye Sensitized Solar Cells Assesed by Density Functional Theory, *Mat. Sci. Semicon. Proc.*, 26, 119-129.
- Shi, J.H., Li, Z., Liu, W.Y., Yu, M., Li, Z.H., and Liu, G.F., 2013, Synthesis and Properties Study of Asymmetrical Carbazole Porphyrin with *p*-hydroxylphenyl and its Metal Complexes (Zn, Dy), *Synth. React. Inorganic, Met. Nano-Metal Chem.*, 43 (3), 316–320.
- Slater, J.C., 1930, Atomic Shielding Constant, *Phys. Rev.*, 36, 57-64.

- Swick, S.M., Zhu, W., Matta, M., Aldrich, T.J., Harbuzaru, A., Navarette, J.T.L., Ortiz, R.P., Kohlstedt, K.L., Schatz, G.C., Facchetti, A., Melkonyan, F.S., and Marks, T.J., 2018, Closely Packed, Low Reorganization Energy π -Extended Postfullerene Acceptor for Efficient Polymer Solar Cells, *Proc. Natl. Acad. Sci. U.S.A.*, 115(36), E8341-E8348.
- Sze and Simon, M., 1981, *Physics of Semiconductor Devices*, 2nd ed., John Wiley and Sons, New York.
- Tai, C.K., Chuang, W.H., and Wang, B.C., 2013, Substituted Group and Side Chain Effects for the Porphyrin and Zinc(II)-Porphyrin Derivatives: A DFT and TD-DFT study, *J. Lumin.*, 142, 8-16.
- Takahashi, J., 2019, Theory of Carrier Accumulation in Organic Heterojunctions, *Org. Electron.*, 65, 26–30.
- Tsuda, M., Dy, E.S., and Kasai, H., 2005, Comparative Study of O₂ Dissociation on Various Metalloporphyrins, *J. Chem. Phys.*, 122, 244719.
- Verma, S. and Ghosh, H.N., 2012, Exciton Energy and Charge Transfer in Porphyrin Aggregate/Semiconductor (TiO₂) Composites, *J. Phys. Chem. Lett.*, 3 (14), 1877–1884.
- Wang, F. and Landau, D.P., 2001, Efficient, Multiple-Range Random Walk Algorithm to Calculate the Density of States, *Phys. Rev. Lett.*, 86, 3250-2053.
- Wilkinson, G., Ston, F.G.A., and Abel, E.W., 1982, *Comprehensive Organometallic Chemistry*, Pergamon Press, Oxford.
- Yedukondalu, M., Maity, D.K., and Ravikanth, M., 2010, β , Meso-Acetylenyl-Bridged, Asymmetrical, Porphyrin Dyads - Synthesis, Spectral, Electrochemical and Computational Studies, *European J. Org. Chem.*, 1544–1561.
- Yu, H.S., Li, S.L., and Truhlar, D.G., 2016, Perspective: Kohn-Sham Density Functional Theory Descending a Staircase, *J. Chem. Phys.*, 145,130901.
- Yu, H.X., Mu, H.M., Zhu, D.R., Zhang, Y., Wang, X.C., and Xiao-An Zhang, S., 2019, DFT Study on the Oxygen Titanium Porphyrin as Sustainable Cyclic Catalyst for Water Splitting, *Int. J. Hydrog. Energy*, 44, 19920–19928.
- Zanatta, A.R., 2019, Revisiting the Optical Bandgap of Semiconductors and the Proposal of a Unified Methodology to its Determination, *Sci. Rep.*, 9, 1–12.
- Zhang, J., Peng, S., Wei, Y., and Zheng, S., 2020, A Theoretical Study of the Absorption Spectra of Electron-Deficient Pentacene Derivatives using DFT and TDDFT, *Spectrochim. Acta Part A Mol. Biomol. Spectrosc.*, 225, 117480.
- Zhuravlyov, S., Rusakova, N., and Korovin, Y., 2008, 4f-Luminescence of Ytterbium Ions in the Complexes with Asymmetric Porphyrins, *J. Alloys. Compd.*, 451 (1), 334-337.