

DAFTAR PUSTAKA

- Ahmad, A. F., Zulkurnain, N., Rosid, S. J. M., Azid, A., Endut, A., Toemen, S., Ismail, S., Abdullah, W. N. W., Aziz, S. M., Yusoff, N. M., Rosid, S. M., and Nasir, N. A., 2022, Catalytic Transesterification of Coconut Oil in Biodiesel Production, *Catal. Surv. from Asia*, 26(3), 129–143.
- Alimova, I., Brito, P., Ribeiro, A., Queiroz, A. M., 2016, *Production of Biodiesel through Esterification Catalysed by Ionic Liquids*, Azerbaijan, Qafqaz University and Polytechnic Institute of Braganca.
- Aradi, B., Hourahine, B., and Frauenheim, T., 2007, DFTB+, a Sparse Matrix-based Implementation of The DFTB Method, *J. Phys. Chem. A*, 111(26), 5678–5684.
- Araya, S. S., Liso, V., Cui, X., Li, N., Zhu, J., Sahlin, S. L., Jensen, S. H., Nielsen, M. P., and Kær, S. K., 2020, A Review of The Methanol Economy: The Fuel Cell Route, *Energy J.*, 13(3), 1-32.
- Ardizzzone, S., Bianchi, C. L., Cappelletti, G., dan Porta, F., 2004, Liquid-Phase Catalytic Activity of Sulfated Zirconia from Sol-Gel Precursors: The Role of The Surface Features, *J. Catal.*, 227(2), 470–478.
- Ariesto, M., Dan, P., dan Widiyatmoko, R., 2017, Simulasi Dinamika Molekular Reaktif Proses Amorfisasi Silikon Kristal, *JusamI*, 18(3), 123-128.
- Bueno, O. V. M., Benítez, J. J., and San-Miguel, M. A., 2020, Elucidating Esterification Reaction During Deposition of Cutin Monomers from Classical Molecular Dynamics Simulations, *J. Mol. Model*, 26(10), 1-10.
- Chen, K., and Zeng, K., 2022, Performance Optimization Model of Molecular Dynamics Simulation Based on Machine Learning and Data Mining Algorithm, *Mob.*, 2022, 1-12.
- Choperena A., Painter P., 2009, Hydrogen Bonding in Polymers: Effect of Temperature on The OH Stretching Bands of Poly(vinylphenol), *Macromolecules*, 42(16), 6159-6165
- Dayrit, F. M., 2015, The Properties of Lauric Acid and Their Significance in Coconut Oil, *JAOCs*, 92(1), 1–15.
- Elstner, M., 2006, The SCC-DFTB Method and Its Application to Biological Systems, *Theor. Chem. Acc.*, 116(1–3), 316–325
- Foresman, J. B., and Frisch, A., 1993, *Exploring Chemistry with Electronic Structure Methods* (2nd ed.), Pittsburg, Gaussian Inc.
- Gang, L., Xinzong, L., and Eli, W., 2007, Solvent-free Esterification Catalyzed by Surfactant-combined Catalysts at Room Temperature, *New J. Chem.*, 31(3), 348–351.

- Gaus, M., Cui, Q., and Elstner, M., 2011, DFTB3: Extension of The Self-Consistent-Charge Density-Functional Tight-Binding Method (SCC-DFTB), *J. Chem. Theory Comput.*, 7(4), 931–948.
- Guo, L., Qi, C., Zheng, X., Zhang, R., Shen, X., and Kaya, S., 2017, Toward Understanding The Adsorption Mechanism of Large Size Organic Corrosion Inhibitors on An Fe(110) Surface using The DFTB Method, *RSC Adv.*, 7(46), 29042–29050.
- Haase, F., and Sauer, J., 1998, The Surface Structure of Sulfated Zirconia: Periodic Ab Initio Study of Sulfuric Acid Adsorbed on $\text{ZrO}_2(101)$ and $\text{ZrO}_2(001)$, *J. Am. Chem. Soc.*, 120(51), 13503–13512.
- Hofmann, A., and Sauer, J., 2004, Surface Structure of Hydroxylated and Sulfated Zirconia. A Periodic Density Functional Study, *J. Phys. Chem. B*, 108(38), 14652–14662.
- Hou, G., Zhu, X., and Cui, Q., 2010, An Implicit Solvent Model for SCC-DFTB with Charge-Dependent Radii, *J. Chem. Theory Comput.*, 6(8), 2303–2314.
- Howard, A. A., Tschumper, G. S., and Hammer, N. I., 2010, Effects of Hydrogen Bonding on Vibrational Normal Modes of Pyrimidine, *J. Phys. Chem. A*, 114(25), 6803–6810.
- Hutama, A. S., Marlina, L. A., Chou, C. P., Irle, S., and Hofer, T. S., 2021, Development of Density-Functional Tight-Binding Parameters for the Molecular Dynamics Simulation of Zirconia, Yttria, and Yttria-Stabilized Zirconia, *ACS Omega*, 6(31), 20530–20548.
- Igawa, N., and Ishii, Y., 2001, Crystal Structure of Metastable Tetragonal Zirconia up to 1473 K, *J. Am. Ceram. Soc.*, 84(5), 1169–1171.
- Kaur, N., and Ali, A., 2015, Preparation and Application of $\text{Ce/ZrO}_2\text{-TiO}_2/\text{SO}_4^{2-}$ as Solid Catalyst for The Esterification of Fatty Acids, *RES*, 81, 421–431.
- Khan, Z., Javed, F., Shamair, Z., Hafeez, A., Fazal, T., Aslam, A., Zimmerman, W. B., and Rehman, F., 2021, Current Developments in Esterification Reaction: A Review on Process and Parameters, *J. Ind. Eng. Chem.*, 103, 80–101.
- Komintarachat, C., and Chuepeng, S., 2010, Methanol-Based Transesterification Optimization of Waste Used Cooking Oil over Potassium Hydroxide Catalyst, *Am. J. Appl. Sci.*, 7(8), 1073–1078.
- Krüger, T., Elstner, M., Schiffels, P., and Frauenheim, T., 2005, Validation of The Density-Functional based Tight-Binding Approximation Method for The Calculation of Reaction Energies and Other Data, *J. Chem. Phys.*, 122(11), 1–5.

- Kuwahara, Y., Fujitani, T., and Yamashita, H., 2014, Esterification of Levulinic Acid with Ethanol over Sulfated Mesoporous zirconosilicates: Influences of The Preparation Conditions on The Structural Properties and Catalytic Performances, *Catal.*, 237, 18–28.
- Lau, D., Jian, W., Yu, Z., and Hui, D., 2018, Nano-Engineering of Construction Materials using Molecular Dynamics Simulations: Prospects and Challenges. In Composites Part B, *Elsevier Eng.*, 143, 282–291.
- Leach, A. R., 2001, *Molecular Modelling Principles and Applications* (2nd ed.), England, Pearson Education.
- Liang, R., Swanson, J. M. J., and Voth, G. A., 2014, Benchmark Study of The SCC-DFTB Approach for a Biomolecular Proton Channel, *J. Chem. Theory Comput.*, 10(1), 451–462.
- Lukeš, V., Rimarčík, J., Rottmannová, L., Punyain, K., Klein, E., and Kelterer, A. M., 2012, On The Applicability of The Molecular Dynamics SCC-DFTB Treatment on Optical Spectra Simulations for Thiophene and Phenyl Containing Oligomers, *Comput. Theor. Chem.*, 999, 55–65.
- Manzhos, S., 2016, Comparative Density Functional Theory and Density Functional Tight Binding Study of 2-Anthroic Acid on TiO₂, *Chem. Phys. Lett.*, 643, 16–20.
- Marutaphan, A., dan Wongchoosuk, C., 2017, SCC-DFTB Study on Structure, Electronic and Sensing Properties of Polypyrrole, *J. Phys. Conf. Ser.*, 901(1), 1-6.
- Murthy, K., 2013, Biodiesel: A Review, *Int. J. Eng. Res.*, 3, 902-912.
- Nakpong, P., and Wootthikanokkhan, S., 2010, High Free Fatty Acid Coconut Oil as a Potential Feedstock for Biodiesel Production in Thailand, *Renewable Energy*, 35(8), 1682–1687.
- Nguyen, D. T., and Pham, Q. T., 2020, A Theoretical and Experimental Study on Esterification of Citric Acid with the Primary Alcohols and the Hydroxyl Groups of Cellulose Chain (n = 1-2) in Parched Condition, *J. Chem.*, 2020, 1-9.
- Nigiz, F. U., 2021, Comparative Study on Use of Pervaporation Membrane Reactor for Lauric Acid-Methanol Esterification, *Sep. Purif. Technol.*, 264, 1-10.
- Omar, W. N. N. W., and Amin, N. A. S., 2011, Optimization of Heterogeneous Biodiesel Production from Waste Cooking Palm Oil via Response Surface Methodology, *Biomass and Bioenerg.*, 35(3), 1329–1338.
- Ootani, Y., and Kubo, M., 2022, Density-Functional Tight-Binding Molecular Dynamics Simulation of the Bending Mechanism of Molecular Crystals, *J. Phys. Chem. C.*, 126(25), 10554–10565.

- Patel, A., Brahmkhatri, V., and Singh, N., 2013, Biodiesel Production by Esterification of Free Fatty Acid over Sulfated Zirconia, *RES*, 51, 227–233.
- Patel, S., Baker, Natalie., Marques, Isabella., Hamlekhan, Azhang., Mathew, Mathew., Takoudis, Christos., Friedrich, Craig., Sukotjo, Cortino., Shokuhfar, Tolou., 2017, Transparent TiO₂ Nanotubes on Zirconia for Biomedical Applications, *RSC Adv.*, 7, 30397-30410.
- Patil, M. K., Prasad, A. N., and Reddy, B. M., 2011, Zirconia-Based Solid Acids: Green and Heterogeneous Catalysts for Organic Synthesis, *Curr. Org. Chem.*, 15, 3961-3985.
- Pirnie, M., 1999, *Evaluation of The Fate and Transport of Methanol In The Environment*, America, Malcolm Pirnie Inc.
- Poulikakos, D., and Maruyama, S., 2003, Review Microscale Thermophysical Engineering, *Nanoscale Microsc. Therm.*, 7(3), 181–206.
- Rabee, A., Mekhemer, G., Osatiashtiani, A., Isaacs, M., Lee, A., Wilson, K., Zaki, M., 2017, Acidity Reactivity Relationships in Catalytic Esterification over Ammonium Sulfate Derived Sulfated Zirconia, *Catalysts*, 7(7), 204.
- Rachmat, A., Trisunaryanti, W., Sutarno, and Wijaya, K., 2017, Synthesis and Characterization of Sulfated Zirconia Mesopore and Its Application on Lauric Acid Esterification, *Mater. Renew. Sustain. Energy*, 6(3), 181-206.
- Sakai, T., Kawashima, A., and Koshikawa, T., 2009, Economic Assessment of Batch Biodiesel Production Processes using Homogeneous and Heterogeneous Alkali Catalysts, *Bioresour. Technol.*, 100(13), 3268–3276.
- Sandhya, S., Talukdar, J., and Bhaishya, D., 2016, Chemical and Biological Properties of Lauric Acid: A Review, *Int. J. Adv. Res. Publ.*, 4(7), 1123–1128.
- Sandoval, G., Casas-Godoy, L., Bonet-Ragel, K., Rodrigues, J., Ferreira-Dias, S., and Valero, F., 2017, Enzyme-Catalyzed Production of Biodiesel as Alternative to Chemical- Catalyzed Processes: Advantages and Constraints, *Curr. Biochem. Eng.*, 4(2), 1-33.
- Saravanan, K., Tyagi, B., and Bajaj, H. C., 2016, Nano-crystalline, Mesoporous Aerogel Sulfated Zirconia as an Efficient Catalyst for Esterification of Stearic Acid with Methanol, *Appl. Catal.*, 192, 161–170.
- Schlegel, H. B., 2011, Geometry Optimization, *Wiley Interdiscip. Rev. Comput. Mol. Sci.*, 1(5), 790–809.

- Sendilvelan, S., and Bhaskar, K., 2017, Chemical and Experimental Analysis of Fumigation Process to Reduce Emission Without Affecting the Performance of an Engine, *Rasayan J. Chem.*, 10(1), 111–116.
- Shankar, S., Agarwal, M., and Chaurasia, S. P., 2013, Study of Reaction Parameters and Kinetics of Esterification of Lauric Acid with Butanol by Immobilized Candida Antarctica Lipase, *Indian J. Biochem. Biophys.*, 50, 570-576.
- Shi, G., Yu, F., Wang, Y., Pan, D., Wang, H., and Li, R., 2016, A Novel One-Pot Synthesis of Tetragonal Sulfated Zirconia Catalyst with High Activity for Biodiesel Production from The Transesterification of Soybean Oil, *Renew. Eng.*, 92, 22–29.
- Southon, P. D., 2015, *Structural Evolution during The Preparation and Heating of Nanophase Zirconia Gels*, Sydney, University of Technology.
- Takase, M., Zhang, M., Feng, W., Chen, Y., Zhao, T., Cobbina, S. J., Yang, L., and Wu, X., 2014, Application of Zirconia Modified with KOH as Heterogeneous Solid Base Catalyst to New Non-Edible Oil for Biodiesel, *Energy Convers. Manag.*, 80, 117–125.
- Yamaguchi, T., 1994, Application of ZrO_2 as A Catalyst and A Catalyst Support, *Catal. Today*, 20, 199-218.
- Zhang, Q., Yang, T., Lei, D., Wang, J., and Zhang, Y., 2020, Efficient Production of Biodiesel from Esterification of Lauric Acid Catalyzed by Ammonium and Silver Co-Doped Phosphotungstic Acid Embedded in a Zirconium Metal-Organic Framework Nanocomposite, *ACS Omega*, 5(22), 12760–12767.
- Zhang, W., Wang, Z., Huang, J., and Jiang, Y., 2021, Zirconia-Based Solid Acid Catalysts for Biomass Conversion, *Energy and Fuels*, 35(11), 9209–9227.