



## DAFTAR PUSTAKA

- Ali, I., Suhail, M., Alothman, Z.A., and Alwarthan, A., 2018, Recent advances in syntheses, properties and applications of TiO<sub>2</sub> nanostructures, *RSC Adv*, 8, 30125–30147.
- Ameta, R., Solanki, M.S., Benjamin, S., and Ameta, S.C., 2018, Photocatalysis,, In, *Advanced Oxidation Processes for Waste Water Treatment*. Elsevier, pp. 135–175.
- Andita, K.R., Kurniawan, R., and Syoufian, A., 2019, Synthesis and Characterization of Cu-Doped Zirconium Titanate as A Potential Visible-Light Responsive Photocatalyst, *Indonesian Journal of Chemistry*, 19, 761.
- Araujo-Lopez, E., Varilla, L.A., Seriani, N., and Montoya, J.A., 2016, TiO<sub>2</sub> anatase's bulk and (001) surface, structural and electronic properties: A DFT study on the importance of Hubbard and van der Waals contributions, *Surf Sci*, 653, 187–196.
- Azuma, M., Hashimoto, K., Hiramoto, M., Watanabe, M., and Sakata, T., 1990, Electrochemical Reduction of Carbon Dioxide on Various Metal Electrodes in Low-Temperature Aqueous KHCO<sub>3</sub> Media, *J Electrochem Soc*, 137, 1772–1778.
- Bai, S., Jiang, J., Zhang, Q., and Xiong, Y., 2015, Steering charge kinetics in photocatalysis: intersection of materials syntheses, characterization techniques and theoretical simulations, *Chem Soc Rev*, 44, 2893–2939.
- Cai Yanjuan, Wang Yuxiong, Wang Hao, and Chen Fangyan, 2016, Graphitic Carbon Nitrides: Modifications and Applications in Environmental Purification, *Progress in Chemistry*, 28, 428–437.
- Capelle, K., 2002, A bird's-eye view of density-functional theory.,
- Devrim, B. and Bozkır, A., 2017, Nanocarriers and Their Potential Application as Antimicrobial Drug Delivery,. In, *Nanostructures for Antimicrobial Therapy*. Elsevier, pp. 169–202.
- Dondi, M., Matteucci, F., and Cruciani, G., 2006, Zirconium titanate ceramic pigments: Crystal structure, optical spectroscopy and technological properties, *J Solid State Chem*, 179, 233–246.
- Fahmi, H., Timothy, L., Robert, H., Vsevolod, V.R., Louis, N., Barry, K.S., and Valery, V.F., 2005, Copper(I)-catalyzed synthesis of azoles. DFT study predict unprecedented reactivity and intermedieates, *J. Am. Chem. Soc.*, 127(1).



- Fawrin, H., Marlina, L.A., Hutama, A.S., and Trisunaryanti, W., 2021, Investigations of the influence of non-metal dopants on the electronic and photocatalytic properties of ZrTiO<sub>4</sub> by density functional theory calculations, *Computational Condensed Matter*, 29, e00607.
- Fedorov, P.P. and Yarotskaya, E.G., 2021, Zirconium dioxide. Review, *Kondensirovannye sredy i mezhfaznye granitsy = Condensed Matter and Interphases*, 23, 169–187.
- Fegade, U.A. and Jethave, G.N., 2021, Photocatalytic reduction of CO<sub>2</sub> in hydrocarbon: A greener approach for energy production,, pp. 871–915.
- Fei, H., Zhao, T., Guo, W., Wang, X., Zhang, J., Fei, Z., Feng, Z., and Liu, G., 2024, Strategies for enhancing activities of typical piezo-photocatalytic material and its applications in environmental remediation: A review, *J Environ Chem Eng*, 12, 111650.
- Flores, E.M., Moreira, M.L., and Piotrowski, M.J., 2020, Structural and Electronic Properties of Bulk ZnX (X = O, S, Se, Te), ZnF<sub>2</sub>, and ZnO/ZnF<sub>2</sub>: A DFT Investigation within PBE, PBE + *U*, and Hybrid HSE Functionals, *J Phys Chem A*, 124, 3778–3785.
- Ganji, P., Chowdari, R.K., and Likozar, B., 2023, Photocatalytic Reduction of Carbon Dioxide to Methanol: Carbonaceous Materials, Kinetics, Industrial Feasibility, and Future Directions, *Energy & Fuels*, 37, 7577–7602.
- Garvie, R.C., Hannink, R.H., and Pascoe, R.T., 1975, Ceramic steel?, *Nature*, 258, 703–704.
- George, A., Solomon, S., Thomas, J.K., and John, A., 2012, Characterizations and electrical properties of ZrTiO<sub>4</sub> ceramic, *Mater Res Bull*, 47, 3141–3147.
- Gharaei, S.K., Abbasnejad, M., and Maezono, R., 2018, Bandgap reduction of photocatalytic TiO<sub>2</sub> nanotube by Cu doping, *Sci Rep*, 8, 14192.
- Goeppert, A., Czaun, M., Jones, J.-P., Surya Prakash, G.K., and Olah, G.A., 2014, Recycling of carbon dioxide to methanol and derived products – closing the loop, *Chem. Soc. Rev.*, 43, 7995–8048.
- Guil-López, R., Mota, N., Llorente, J., Millán, E., Pawelec, B., Fierro, J.L.G., and Navarro, R.M., 2019, Methanol Synthesis from CO<sub>2</sub>: A Review of the Latest Developments in Heterogeneous Catalysis, *Materials*, 12, 3902.
- Haider, T.P., Völker, C., Kramm, J., Landfester, K., and Wurm, F.R., 2019, Plastics of the Future? The Impact of Biodegradable Polymers on the Environment and on Society, *Angewandte Chemie International Edition*, 58, 50–62.



- Hannink, R.H.J., Kelly, P.M., and Muddle, B.C., 2000, Transformation Toughening in Zirconia-Containing Ceramics, *Journal of the American Ceramic Society*, 83, 461–487.
- Hayati, R., Kurniawan, R., Prasetyo, N., Sudiono, S., and Syoufian, A., 2022, Codoping Effect of Nitrogen (N) to Iron (Fe) Doped Zirconium Titanate (ZrTiO<sub>4</sub>) Composite toward Its Visible Light Responsiveness as Photocatalysts, *Indonesian Journal of Chemistry*, 22, 692.
- Hoffmann, M.R., Martin, S.T., Choi, W., and Bahnemann, D.W., 1995, Environmental Applications of Semiconductor Photocatalysis, *Chem Rev*, 95, 69–96.
- Inoue, T., Fujishima, A., Konishi, S., and Honda, K., 1979, Photoelectrocatalytic reduction of carbon dioxide in aqueous suspensions of semiconductor powders, *Nature*, 277, 637–638.
- Ishida, H. and Sakaba, A., 2017, Temperature dependence of photocatalytic CO<sub>2</sub> reduction by trans(Cl)-Ru(bpy)(CO)<sub>2</sub>Cl<sub>2</sub>: activation energy difference between CO and formate production, *Faraday Discuss*, 198, 263–277.
- Jadhav, S.G., Vaidya, P.D., Bhanage, B.M., and Joshi, J.B., 2014, Catalytic carbon dioxide hydrogenation to methanol: A review of recent studies, *Chemical Engineering Research and Design*, 92, 2557–2567.
- Karunakaran, C. and Dhanalakshmi, R., 2008, Semiconductor-catalyzed degradation of phenols with sunlight, *Solar Energy Materials and Solar Cells*, 92, 1315–1321.
- Lei, Y., Wang, Z., Bao, A., Tang, X., Huang, X., Yi, H., Zhao, S., Sun, T., Wang, J., and Gao, F., 2023, Recent advances on electrocatalytic CO<sub>2</sub> reduction to resources: Target products, reaction pathways and typical catalysts, *Chemical Engineering Journal*, 453, 139663.
- Li, K., Zhang, S., Tan, Q., Wu, X., Li, Y., Li, Q., Fan, J., and Lv, K., 2021, Insulator in photocatalysis: Essential roles and activation strategies, *Chemical Engineering Journal*, 426, 130772.
- Manicone, P.F., Rossi Iommelli, P., and Raffaelli, L., 2007, An overview of zirconia ceramics: Basic properties and clinical applications, *J Dent*, 35, 819–826.
- Mohtar, S.S., Aziz, F., Ismail, A.F., Sambudi, N.S., Abdullah, H., Rosli, A.N., and Ohtani, B., 2021, Impact of Doping and Additive Applications on Photocatalyst Textural Properties in Removing Organic Pollutants: A Review, *Catalysts*, 11, 1160.



- Mosey, N.J. and Carter, E.A., 2007, *Ab initio* evaluation of Coulomb and exchange parameters for DFT+U calculations, *Phys Rev B*, 76, 155123.
- Mulwa, W.M., Ouma, C.N.M., Onani, M.O., and Dejene, F.B., 2016, Energetic, electronic and optical properties of lanthanide doped TiO<sub>2</sub>: An ab initio LDA+U study, *J Solid State Chem*, 237, 129–137.
- Nagaveni, K., Sivalingam, G., Hegde, M.S., and Madras, G., 2004, Solar photocatalytic degradation of dyes: high activity of combustion synthesized nano TiO<sub>2</sub>, *Appl Catal B*, 48, 83–93.
- Norris, D.J., Efros, A.L., and Erwin, S.C., 2008, Doped Nanocrystals, *Science (1979)*, 319, 1776–1779.
- Nunes, L.J.R., 2023, The Rising Threat of Atmospheric CO<sub>2</sub>: A Review on the Causes, Impacts, and Mitigation Strategies, *Environments*, 10, 66.
- Oanh, L.M., Do, D.B., Hung, N.M., Thang, D.V., Phuong, D.T., Ha, D.T., and Van Minh, N., 2016, Formation of Crystal Structure of Zirconium Titanate ZrTiO<sub>4</sub> Powders Prepared by Sol–Gel Method, *J Electron Mater*, 45, 2553–2558.
- Polliotto, V., Albanese, E., Livraghi, S., Indyka, P., Sojka, Z., Pacchioni, G., and Giamello, E., 2017, Fifty-Fifty Zr-Ti Solid Solution with a TiO<sub>2</sub>-Type Structure: Electronic Structure and Photochemical Properties of Zirconium Titanate ZrTiO<sub>4</sub>, *Journal of Physical Chemistry C*, 121, 5487–5497.
- Puigdollers, A.R., Illas, F., and Pacchioni, G., 2016, Structure and Properties of Zirconia Nanoparticles from Density Functional Theory Calculations, *The Journal of Physical Chemistry C*, 120, 4392–4402.
- Roongcharoen, T., Poobordin, M., Thanadol, J., Pornsawan, S., Teera, B., Kaito, T., Supawadee, N., 2022, Theoretical insight on why N-vacancy promotes the selective CO<sub>2</sub> reduction to ethanol on NiMn doped graphitic carbon nitride sheets, *App. Sur. Sci.*, 153527.
- Reddy, B.M. and Khan, A., 2005, Recent Advances on TiO<sub>2</sub>-ZrO<sub>2</sub> Mixed Oxides as Catalysts and Catalyst Supports, *Catalysis Reviews*, 47, 257–296.
- Saravanan, R., Francisco, G., and Stephen, A., 2017, Basic Principles, Mechanism, and Challenges of Photocatalysis, *SSPCM*, 19 – 40.
- Shokri, A., Yazdani, A., and Rahimi, K., 2020, Possible bandgap values of graphene-like ZnO in density functional theory corrected by the Hubbard U term and HSE hybrid functional, *Mater Today Commun*, 22, 100756.



- Singh, M.R., Kwon, Y., Lum, Y., Ager, J.W., and Bell, A.T., 2016, Hydrolysis of Electrolyte Cations Enhances the Electrochemical Reduction of CO<sub>2</sub> over Ag and Cu, *J Am Chem Soc*, 138, 13006–13012.
- Singh, P. and Harbola, M.K., 2020, Density-functional theory of material design: fundamentals and applications-I, *Oxford Open Materials Science*, 1.
- Troitzsch, U., Christy, A.G., and Ellis, D.J., 2007, Synthesis of zirconium titanate with an ordered M-fergusonite (beta) structure, *J Solid State Chem*, 180, 2885–2895.
- Troitzsch, U. and Ellis, D.J., 2005, The ZrO<sub>2</sub>-TiO<sub>2</sub> phase diagram, *J Mater Sci*, 40, 4571–4577.
- Umezawa, N. and Ye, J., 2012, Role of complex defects in photocatalytic activities of nitrogen-doped anatase TiO<sub>2</sub>, *Physical Chemistry Chemical Physics*, 14, 5924.
- Varela, A.S., Kroschel, M., Leonard, N.D., Ju, W., Steinberg, J., Bagger, A., Rossmeisl, J., and Strasser, P., 2018, pH Effects on the Selectivity of the Electrocatalytic CO<sub>2</sub> Reduction on Graphene-Embedded Fe-N-C Motifs: Bridging Concepts between Molecular Homogeneous and Solid-State Heterogeneous Catalysis, *ACS Energy Lett*, 3, 812–817.
- Varela, A.S., Kroschel, M., Reier, T., and Strasser, P., 2016, Controlling the selectivity of CO<sub>2</sub> electroreduction on copper: The effect of the electrolyte concentration and the importance of the local pH, *Catal Today*, 260, 8–13.
- Verma, C., Quadri, T.W., Ebenso, E.E., and Quraishi, M.A., 2021, Polymer nanocomposites as industrially useful corrosion inhibitors: recent developments., In, *Handbook of Polymer Nanocomposites for Industrial Applications*. Elsevier, pp. 419–435.
- Vidya, Y.S. and Manjunatha, H.C., 2023, Zirconium titanate nanoparticles: Brief review on the synthesis, *Inorg Chem Commun*, 153, 110772.
- Wang, M., Wang, C., Liu, Y., and Zhou, X., 2019, Hybrid density functional theory description of non-metal doping in perovskite BaTiO<sub>3</sub> for visible-light photocatalysis, *J Solid State Chem*, 280, 121018.
- Wu, H.-C., Lin, S.-W., and Wu, J.-S., 2012, Effects of nitrogen concentration on N-doped anatase TiO<sub>2</sub>: Density functional theory and Hubbard U analysis, *J Alloys Compd*, 522, 46–50.
- Yalçın, Y., Kılıç, M., and Çınar, Z., 2010, The Role of Non-Metal Doping in TiO<sub>2</sub> Photocatalysis, *Journal of Advanced Oxidation Technologies*, 13, .



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Studi Reduksi CO<sub>2</sub> Menjadi CH<sub>3</sub>OH Melalui Jalur Karboksil Pada Permukaan ZrTiO<sub>4</sub> (111) Terdoping Sulfur  
Dengan Teori Fungsi Kerapatan  
WAFA' DZOFARI HILMY, Dr. Sc. Aulia Sukma Hutama, S.Si., M.Si.

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Zhang, H. and Banfield, J.F., 2000, Understanding Polymorphic Phase Transformation Behavior during Growth of Nanocrystalline Aggregates: Insights from TiO<sub>2</sub>, *J Phys Chem B*, 104, 3481–3487.

Zhao, Y., Lin, Y., Wang, G., Jiang, Z., Zhang, R., and Zhu, C., 2018, Electronic and optical performances of (Cu, N) codoped TiO<sub>2</sub>/g-C3N4 heterostructure photocatalyst: A spin-polarized DFT + U study, *Solar Energy*, 162, 306–316.