

DAFTAR PUSTAKA

- Al-Hamdani, Y.S., Michaelides, A., and Von Lilienfeld, O.A., 2017, Exploring dissociative water adsorption on isoelectronically BN doped graphene using alchemical derivatives, *J. Chem. Phys.*, 147, .
- Alam, M., Rahman, A., Alandis, N., and Shaik, M.R., 2013, Report on Selective Acylation of Benzylic Alcohol to Benzyl Acetate with Catalytic System Ni/SiO₂: An Environmentally Benevolent Approach, *Oxid. Commun.*, 36, 261–270.
- Alam, M., Rahman, A., Alandis, N.M., and Shaik, M.R., 2013, Report on selective acylation of benzylic alcohol to benzyl acetate with catalytic system ni/sio₂: An environmentally benevolent approach, *Oxid. Commun.*, 36, 261–270.
- An, D., Guo, Y., Zhu, Y., and Wang, Z., 2010, A green route to preparation of silica powders with rice husk ash and waste gas, *Chem. Eng. J.*, 162, 509–514.
- Anderson, R.J., Bendell, D.J., and Groundwater, P.W., 2004, Organic Spectroscopy Analysis, Bendell, D.J. and Groundwater, P.W. (eds) Royal Society of Chemistry, Great Britain.
- Azat, S., Sartova, Z., Bekseitova, K., and Askaruly, K., 2019, Extraction of high-purity silica from rice husk via hydrochloric acid leaching treatment, *Turkish J. Chem.*, 43, 1258–1269.
- Badoei-dalfard, A., Tahami, A., and Karami, Z., 2022, Lipase immobilization on glutaraldehyde activated graphene oxide/chitosan/cellulose acetate electrospun nanofibrous membranes and its application on the synthesis of benzyl acetate, *Colloids Surfaces B Biointerfaces*, 209, 112151.
- Bahamon, D., Khalil, M., Belabbes, A., Alwahedi, Y., Vega, L.F., and Polychronopoulou, K., 2021, A DFT study of the adsorption energy and electronic interactions of the SO₂ molecule on a CoP hydrotreating catalyst, *RSC Adv.*, 11, 2947–2957.
- Bakar, R.A., Yahya, R., and Gan, S.N., 2016, Production of High Purity Amorphous Silica from Rice Husk, *Procedia Chem.*, 19, 189–195.
- Bass, J.D., Solovyov, A., Pascall, A.J., and Katz, A., 2006, Acid-base bifunctional and dielectric outer-sphere effects in heterogeneous catalysis: A comparative investigation of model primary amine catalysts, *J. Am. Chem. Soc.*, 128, 3737–3747.
- Basu, P., Bhanja, P., Salam, N., Dey, T.K., Bhaumik, A., Das, D., and Islam, S.M., 2017, Silver nanoparticles supported over Al₂O₃@Fe₂O₃ core-shell nanoparticles as an efficient catalyst for one-pot synthesis of 1,2,3-triazoles and acylation of benzyl alcohol, *Mol. Catal.*, 439, 31–40.
- Budiman, A.W., Qurrotul'aini, N. 'Abidah, Latifah, N., Dewani, P.H.,

- Rachmadhani, S., and Wigati, S.M., 2022, The Effects of Different Nickel–Ruthenium on SiO₂ Catalyst Synthesis Methods toward Catalytic Activity of Methane Dry Reforming, *Equilib. J. Chem. Eng.*, 5, 67–74.
- Chmielarz, L. and Aleksandra, J., 2021, Mesoporous silica-based catalysts for selective catalytic reduction of NO_x with ammonia—Recent advances, *Adv. Inorg. Chem.*, 79, 209–245.
- Cueto-Díaz, E.J., Castro-Muñiz, A., Suárez-García, F., Gálvez-Martínez, S., Torquemada-Vico, M.C., Valles-González, M.P., and Mateo-Martí, E., 2021, APTES-Based Silica Nanoparticles as a Potential Modifier for the Selective Sequestration of CO₂ Gas Molecules, *Nanomaterials*, 11, .
- D’Souza, J. and Nagaraju, N., 2006, Catalytic activity of anion-modified zirconia, alumina and silica in the esterification of benzyl alcohol with acetic acid, *Indian J. Chem. Technol.*, 13, 605–613.
- Daffalla, S.B., Mukhtar, H., and Shaharun, M.S., 2020, Preparation and characterization of rice husk adsorbents for phenol removal from aqueous systems, *PLoS One*, 15, .
- Demirörs, A.F., Van Blaaderen, A., and Imhof, A., 2009, Synthesis of eccentric titania-silica core-shell and composite particles, *Chem. Mater.*, 21, 979–984.
- Dhaneswara, D., Fatriansyah, J.F., Situmorang, F.W., and Nurul, A., 2020, Synthesis of Amorphous Silica from Rice Husk Ash: Comparing HCl and CH₃COOH Acidification Methods and Various Alkaline Concentrations, *Int. J. Technol.*, 11, 200–208.
- Díaz-Sánchez, M., Diana Díaz-García, ., Sanjiv Prashar, ., and Santiago Gómez-Ruiz, ., 2019, Palladium nanoparticles supported on silica, alumina or titania: greener alternatives for Suzuki-Miyaura and other C-C coupling reactions, *Environ. Chem. Lett.*, 17, 1585–1602.
- Duong, A.N., Wang, B., Sooknoi, T., Steven, P., Resasco, D.E., Duong, N.N., Wang, B., Sooknoi, T., Crossley, S.P., and Resasco, D.E., 2017, Enhancing the Acylation Activity of Acetic Acid by Forming an Intermediate Aromatic Ester, *ChemSusChem*, 10, 2823–2832.
- Ebrahimi, J., Ahangari, M.G., and Jahanshahi, M., 2018, Computational studies at the density functional theory (DFT) level about the surface functionalization of hexagonal monolayers by chitosan monomer, *Appl. Surf. Sci.*, 440, 778–789.
- El-Sayed, A.M., Watkins, M.B., Shluger, A.L., and Afanas’Ev, V. V., 2013, Identification of intrinsic electron trapping sites in bulk amorphous silica from ab initio calculations, *Microelectron. Eng.*, 109, 68–71.
- Faé Gomes, G.M., Philipssen, C., Bard, E.K., Zen, L.D., and De Souza, G., 2016, Rice husk bubbling fluidized bed combustion for amorphous silica synthesis, *J. Environ. Chem. Eng.*, 4, 2278–2290.

- Fathi Vavsari, V., Mohammadi Ziarani, G., Badiei, A., and Balalaie, S., 2016, Application of SBA-Pr-SO₃H as a nanoreactor in the one-pot synthesis of spiroquinazolinones, *J. Iran. Chem. Soc.*, 13, 1037–1043.
- Fortea-Pérez, F.R., Vallejo, J., Mastropietro, T.F., Munno, G. De, Rabelo, R., Cano, J., and Julve, M., 2023, Field-Induced Single-Ion Magnet Behavior in Nickel(II) Complexes with Functionalized 2,2':6'-2''-Terpyridine Derivatives: Preparation and Magneto-Structural Study, *Molecule*, 28, .
- Garofalini, S.H., 1983, A molecular dynamics simulation of the vitreous silica surface, *J. Chem. Phys.*, 78, 4–8.
- Glossman-Mitnik, D., 2022, Density Functional Theory: Recent Advances, New Perspective and Applications, IntechOpen, London.
- Glover, T.G. and Mu, B. eds., 2018, Gas Adsorption in Metal-Organic Frameworks: Fundamentals and Applications, CRC Press, New York.
- Gomes, E.O., Fabris, G.S.L., Ferrer, M.M., Motta, F. V., Bomio, M.R.D., Andres, J., Longo, E., and Sambrano, J.R., 2019, Computational procedure to an accurate DFT simulation to solid state systems, *Comput. Mater. Sci.*, 170, 109176.
- Hagen, J., 2006, Industrial Catalysis: A Practical Approach, 2nd ed. Wiley-VCH, Weinheim.
- Hossain, S.K.S., Mathur, L., Roy, P.K., Hossain, S.K.S., Mathur, L., and Rice, P.K.R., 2018, Rice husk / rice husk ash as an alternative source of silica in ceramics : A review, *J. Asian Ceram. Soc.*, 6, 299–313.
- Iqbal, J. and Srivastava, R.R., 1992, Cobalt (II) Chloride Catalyzed Acylation of Alcohols with Acetic Anhydride : Scope and Mechanism, *J. Org. Chem.*, 57, 2001–2007.
- Isasi, J., Arevalo, P., Martin, E., and Martín-Hernández, F., 2019, Preparation and study of silica and APTES – silica-modified NiFe₂O₄ nanocomposites for removal of Cu²⁺ and Zn²⁺ ions from aqueous solutions, *J. Sol-Gel Sci. Technol.*, 91, 596–610.
- Jamwal, B., Kaur, M., Sharma, H., Khajuria, C., Paul, S., and Clark, J.H., 2019, Diamines as interparticle linkers for silica-titania supported PdCu bimetallic nanoparticles in Chan-Lam and Suzuki cross-coupling reactions, *New J. Chem.*, 43, 4919–4928.
- Jeong, U., Shin, H.H., and Kim, Y., 2015, Functionalized magnetic core–shell Fe@SiO₂ nanoparticles as recoverable colorimetric sensor for Co²⁺ ion, *Chem. Eng. J.*, 281, 428–433.
- Khajehzadeh, M. and Moghadam, M., 2018, A new poly(N–heterocyclic carbene Pd complex) immobilized on nano silica: An efficient and reusable catalyst for Suzuki–Miyaura, Sonogashira and Heck–Mizoroki C–C coupling reactions, *J.*

Organomet. Chem., 863, 60–69.

Kurth, S., Marques, M.A.L., and Gross, E.K.U., 2005, Density-Functional Theory, *Encycl. Condens. Matter Phys.*, 395–402.

Kusumaningtyas, D.T., Prasetyoko, D., Suprpto, S., and Triwahyono, S., 2017, Esterification of Benzyl Alcohol with Acetic Acid over Mesoporous H-ZSM-5,12, 243–250.

Kwan, W.H. and Wong, Y.S., 2020, Acid leached rice husk ash (ARHA) in concrete: A review, *Mater. Sci. Energy Technol.*, 3, 501–507.

Li, J.F., Wang, Y.F., Wu, Y.Y., Liu, W.J., and Wang, J.W., 2020, Nickel - Catalyzed Esterification of Amides Under Mild Conditions, *Catal. Letters*, 150, 874–880.

Li, N. and Ching, W.Y., 2014, Structural, electronic and optical properties of a large random network model of amorphous SiO₂ glass, *J. Non. Cryst. Solids*, 383, 28–32.

Liu, S.H., 2014, Catalytic Synthesis of Benzyl Acetate by Diatomite Supported Waugh-Type (NH₄)₆[MnMo₉O₃₂] • 8H₂O, *Appl. Mech. Mater.*, 483, 38–41.

Mahdian, S., Naimi-Jamal, M.R., and Panahi, L., 2018, Activity of M₂(BDC)₂(DABCO) (M= Co, Ni, Cu and Zn) Metal-Organic Frameworks Prepared via Ball-Milling Solvent-Free Method in Acylation of Alcohols, Amines and Aldehydes, *ChemistrySelect*, 3, 11223–11229.

Mandal, P., Molla, R.A., Chattopadhyay, A.P., Poddar, S., and Biswas, H.S., 2022, GO-APTES-Cu (II) Schiff base complex as efficient heterogeneous catalyst for aerobic decarboxylation reaction of phenylacetic acids, *Inorg. Chem. Commun.*, 144, 1–22.

Mandal, S., Roy, D., Chaudhari, R. V., and Sastry, M., 2004, Pt and Pd nanoparticles immobilized on amine-functionalized zeolite: Excellent catalysts for hydrogenation and heck reactions, *Chem. Mater.*, 16, 3714–3724.

Masoud, S.-N., Tahereh, K., and Samansa, H., 2005, Highly selective esterification of tert-butanol by acetic acid anhydride over alumina-supported InCl₃, GaCl₃, FeCl₃, ZnCl₂, CuCl₂, NiCl₂, CoCl₂ and MnCl₂ catalysts, *J. Mol. Catal. A Chem.*, 235, 150–153.

Mekrattanachai, P., Zhu, L., Setthaya, N., Chindawong, C., and Guo, W., 2022, The Highly Effective Cobalt Based Metal – Organic Frameworks Catalyst for One Pot Oxidative Esterification Under Mild Conditions, *Catal. Letters*, 152, 1639–1650.

Meshram, G. and Patil, V.D., 2009, Simple and efficient method for acetylation of alcohols, phenols, amines, and thiols using anhydrous NiCl₂ under solvent-free conditions, *Synth. Commun.*, 39, 4384–4395.

Minchitha, U.K., Hareesh, N.H., Nagaraju, N., and Kathyayini, H., 2016, Catalytic

activity studies of modified alumina in the esterification of benzyl alcohol with different aliphatic acids, *J. Sci. Ind. Res. (India)*, 75, 244–252.

- Modak, A., Mondal, J., and Bhaumik, A., 2012, Pd-grafted periodic mesoporous organosilica: An efficient heterogeneous catalyst for Hiyama and Sonogashira couplings, and cyanation reactions, *Green Chem.*, 14, 2840–2855.
- Moreno, J.J.G., Pan, K., Wang, Y., and Li, W., 2020, Computational Study of APTES Surface Functionalization of Diatom-like Amorphous SiO₂ Surfaces for Heavy Metal Adsorption, *ChemRxiv*, 36, 5680–5689.
- Mourik, T. Van, Bühl, M., and Gaigeot, M.-P., 2014, Density Functional Theory Across Chemistry, Physics and Biology, *Philos. Trans. R. Soc. A*, 372, .
- Mulla, S.A.R., Inamdar, S.M., Pathan, M.Y., and Chavan, S.S., 2012, Highly Efficient Cobalt (II) Catalyzed O-Acylation of Alcohols and Phenols under Solvent-Free Conditions, *Open J. Synth. Theory Appl.*, 01, 31–35.
- Neiman, M.L.L., 2003, Interaction of Cobalt and Nickel with the Hydroxylated Silanol Silica Surface: A Theoretical Study, .
- Nie, W., Luo, Y., Yang, Q., Feng, G., Yao, Q., and Lu, Z.H., 2020, An amine-functionalized mesoporous silica-supported pdir catalyst: Boosting room-temperature hydrogen generation from formic acid, *Inorg. Chem. Front.*, 7, 709–717.
- Nikoorazm, M., Ghorbani-Choghamarani, A., Noori, N., and Tahmasbi, B., 2016, Palladium 2-mercapto-N-propylacetamide complex anchored onto MCM-41 as efficient and reusable nanocatalyst for Suzuki, Stille and Heck reactions and amination of aryl halides, *Appl. Organomet. Chem.*, 30, 843–851.
- Onwuka, J.C., Agbaji, E.B., Ajibola, V.O., and Okibe, F.G., 2019, Thermodynamic pathway of lignocellulosic acetylation process, *BMC Chem.*, 13, 1–11.
- Oosthoek-De Vries, A.J., Nieuwland, P.J., Bart, J., Koch, K., Janssen, J.W.G., Van Bentum, P.J.M., Rutjes, F.P.J.T., Gardeniers, H.J.G.E., and Kentgens, A.P.M., 2019, Inline Reaction Monitoring of Amine-Catalyzed Acetylation of Benzyl Alcohol Using a Microfluidic Stripline Nuclear Magnetic Resonance Setup, *J. Am. Chem. Soc.*, 141, 5369–5380.
- Patel, A.R., Asatkar, A., Patel, G., and Banerjee, S., 2019, Synthesis of Rice Husk Derived Activated Mesoporous Carbon Immobilized Palladium Hybrid Nano-Catalyst for Ligand-Free Mizoroki-Heck/Suzuki/Sonogashira Cross-Coupling Reactions, *ChemistrySelect*, 4, 5577–5584.
- Pieber, B., Malik, J.A., Cavedon, C., Gisbertz, S., Savateev, A., Cruz, D., Heil, T., Zhang, G., Seeberger, P.H., Pieber, B., Malik, J.A., Cavedon, C., and Gisbertz, S., 2019, Semi-Heterogeneous Dual Nickel/Photocatalysis using Carbon Nitrides: Esterification of Carboxylic Acids with Aryl Halides Semi-Heterogeneous Dual Nickel/Photocatalysis using Carbon Nitrides: Esterification of Carboxylic Acids with Aryl Halides, *Angew. Chemie*, 58,

9575–9580.

- Qiao, B., Wang, T.J., Gao, H., and Jin, Y., 2015, High density silanization of nano-silica particles using γ -aminopropyltriethoxysilane (APTES), *Appl. Surf. Sci.*, 351, 646–654.
- Qiao, Z.A. and Huo, Q.S., 2017, *Synthetic Chemistry of the Inorganic Ordered Porous Materials*, Elsevier B.V.
- Rajabi, F., 2009, A heterogeneous cobalt(II) Salen complex as an efficient and reusable catalyst for acetylation of alcohols and phenols, *Tetrahedron Lett.*, 50, 395–397.
- Ramirez, I.A.G., Varilla, L.A.A., and Montoya, J.A., 2019, A DFT study about the effects of exchange-correlation functional on the structural and electronic properties of Anatase, *J. Phys. Conf. Ser.*, 1219, .
- Ren, D., Xiang, B., Hu, C., Qian, K., and Cheng, X., 2018, The electronic and optical properties of amorphous silica with hydrogen defects by ab initio calculations, *J. Semicond.*, 39, .
- Rösler, S., Ertl, M., Irrgang, T., and Kempe, R., 2015, Cobalt-Catalyzed Alkylation of Aromatic Amines by Alcohols, *Angew. Chemie Int. Ed.*, 54, 15046–15050.
- Sadeq, Z.E., Al-Obaidi, N.S., Hammoodi, O.G., Abd, A.N., and Al-Mahdawi, A.S., 2022, Benzyl Acetate: A Review on Synthetic Methods, *Eurasian J. Physics, Chem. Math.*, 9, 28–36.
- Sarkar, S.M., Rahman, M.L., and Yusoff, M.M., 2015, Highly active thiol-functionalized SBA-15 supported palladium catalyst for Sonogashira and Suzuki-Miyaura cross-coupling reactions, *RSC Adv.*, 5, 1295–1300.
- Satya, P., Tuli, G.D., Basu, S.K., and Madan, R., 2022, *Advanced Inorganic Chemistry Volume I (LPSPE)*, S Chand, New Delhi.
- Sawant, D.P., Vinu, A., Justus, J., Srinivasu, P., and Halligudi, S.B., 2007, Catalytic performances of silicotungstic acid/zirconia supported SBA-15 in an esterification of benzyl alcohol with acetic acid, *J. Mol. Catal. A Chem.*, 276, 150–157.
- Setyawan, N., Hoerudin, and Yuliani, S., 2021, Synthesis of silica from rice husk by sol-gel method, *IOP Conf. Ser. Earth Environ. Sci.*, 733, .
- Sholl, D.S. and Steckel, J.A., 2023, *Density Functional Theory A Practical Introduction*, 2nd ed. John Wiley & Sons, Inc., New Jersey.
- Singhal, A., 2009, *Objective Chemistry for the AIEEE*, Pearson Education, New Delhi.
- Siswanta, D. and Nugraha, G., 2017, Pemodelan dan Analisis QSAR Turunan Aminosulfenil Metilkarbamat sebagai Insektisida menggunakan Metode Semiempirik Austin Model 1, *ALKIMIA J. Ilmu Kim. dan Terap.*, 1, 43–49.

- Smith, M.B., 2016, *Organic Chemistry: An Acid-Base Approach*, 2nd ed. CRC Press, Boca Raton.
- Sonawane, R.B., Sonawane, S.R., Rasal, N.K., and Jagtap, S. V., 2020, Chemoselective: O -formyl and O -acyl protection of alkanolamines, phenoxyethanols and alcohols catalyzed by nickel(ii) and copper(ii)-catalysts, *Green Chem.*, 22, 3186–3195.
- Song, S., Cho, H.B., and Kim, H.T., 2018, Surfactant-free synthesis of high surface area silica nanoparticles derived from rice husks by employing the Taguchi approach, *J. Ind. Eng. Chem.*, 61, 281–287.
- Uozumi, Y., Matsuura, Y., Arakawa, T., and Yamada, Y.M.A., 2009, Asymmetric Suzuki–Miyaura Coupling in Water with a Chiral Palladium Catalyst Supported on an Amphiphilic Resin, *Angew. Chemie Int. Ed.*, 48, 2708–2710.
- Usgodaarachchi, L., Thambiliyagodage, C., Wijesekera, R., and Bakker, M.G., 2021, Current Research in Green and Sustainable Chemistry Synthesis of mesoporous silica nanoparticles derived from rice husk and surface-controlled amine functionalization for efficient adsorption of methylene blue from aqueous solution, *Curr. Res. Green Sustain. Chem.*, 4, 100116.
- Vayghan, A.G., Khaloo, A.R., and Rajabipour, F., 2013, The effects of a hydrochloric acid pre-treatment on the physicochemical properties and pozzolanic performance of rice husk ash, *Cem. Concr. Compos.*, 39, 131–140.
- Velusamy, S., Borpuzari, S., and Punniyamurthy, T., 2005, Cobalt(II)-catalyzed direct acetylation of alcohols with acetic acid, *Tetrahedron*, 61, 2011–2015.
- Vladilo, G. and Hassanali, A., 2018, Hydrogen bonds and life in the universe, *Life*, 8, 1–22.
- Wang, G., Li, Z., Li, C., and Zhang, S., 2018, Cobalt catalyzed synthesis of a, b -unsaturated esters from esters and alcohols via mild O₂-interrupted hydrogen borrowing, *J. Catal.*, 368, 228–236.
- Wei, Y., Yang, W., and Yang, Z., 2022, An excellent universal catalyst support-mesoporous silica: Preparation, modification and applications in energy-related reactions, *Int. J. Hydrogen Energy*, 47, 9537–9565.
- Weires, N.A., Caspi, D.D., and Garg, N.K., 2017, Kinetic Modeling of the Nickel-Catalyzed Esterification of Amides, *ACS Catal.*, 7, 4381–4385.
- Widiyandari, H., Pardoyo, P., Sartika, J., Putra, O.A., Purwanto, A., and Ernawati, L., 2021, Synthesis of mesoporous SiO₂ xerogel from geothermal sludge using sulfuric acid as gelation agent, *Int. J. Eng. Trans. A Basics*, 34, 1569–1575.
- Xia, W., 2016, Interactions between metal species and nitrogen-functionalized carbon nanotubes, *Catal. Sci. Technol.*, 6, 630–644.
- Xie, X., He, C., Li, B., He, Y., Cullen, D.A., Wegener, E.C., Kropf, A.J., Martinez, U., Cheng, Y., Engelhard, M.H., Bowden, M.E., Song, M., Lemmon, T., Li,



UNIVERSITAS
GADJAH MADA

Imobilisasi Ni(II) dan Co(II) pada Silika Mesopori Terfungsionalisasi Amina sebagai Katalis dalam Reaksi Asetilasi Benzil Alkohol

Wardah Nabilah, Prof. Dra. Eko Sri Kunarti, M.Si., Ph.D.; Fajar Inggit Pambudi, S.Si., M.Sc., Ph.D.

Universitas Gadjah Mada, 2023 | Diunduh dari <http://etd.repository.ugm.ac.id/>

X.S., Nie, Z., Liu, J., Myers, D.J., Zelenay, P., Wang, G., et al., 2020, Performance enhancement and degradation mechanism identification of a single-atom Co–N–C catalyst for proton exchange membrane fuel cells, *Nat. Catal.*, 3, 1044–1054.