

## DAFTAR PUSTAKA

- Akiba, E., 1999, Hydrogen-Absorbing Alloys. *Curr. Opin. Solid State Mater. Sci.*, 4(3), 267-272.
- Amrhar, O., El Gana, L., and Mobarak, M., 2021, Calculation of Adsorption Isotherms by Statistical Physics Models: A Review, *Environ. Chem. Lett.*, 19(6), 4519-4547.
- Atashrouz, S. and Rahmani, M., 2020, Predicting Hydrogen Storage Capacity of Metal–Organic Frameworks Using Group Method of Data Handling, *Neural Comput. Appl.*, 32(18), 14851-14864.
- Bakowies, D., 2019, Estimating Systematic Error and Uncertainty in Ab Initio Thermochemistry: II. ATOMIC(hc) Enthalpies of Formation for a Large Set of Hydrocarbons, *J. Chem. Theory Comput.*, 16(1), 399-426.
- Barman, S., Furukawa, H., Blacque, O., Venkatesan, K., Yaghi, O. M., and Berke, H., 2010, Azulene Based Metal–Organic Frameworks for Strong Adsorption of H<sub>2</sub>, *Chem. comm.*, 46(42), 7981-7983.
- Barman, S., Khutia, A., Koitz, R., Blacque, O., Furukawa, H., Iannuzzi, M., Yaghi, O.M., Janiak, C., Hutter, J., and Berke, H., 2014, Synthesis and Hydrogen Adsorption Properties of Internally Polarized 2, 6-Azulenadicarboxylate Based Metal–Organic Frameworks, *J. Mater. Chem. A*, 2(44), 18823-18830.
- Belof, J. L., Stern, A. C., Eddaoudi, M., and Space, B., 2007, On The Mechanism of Hydrogen Storage in A Metal–Organic Framework Material, *J. Am. Chem. Soc.*, 129(49), 15202-15210.
- Biniwale, R.B., Rayalu, S., Devotta, S., and Ichikawa, M., 2008, Chemical Hydrides: A Solution to High Capacity Hydrogen Storage and Supply, *Int. J. Hydrogen Energy*, 33:360–365
- Biserčić, M. S., Marjanović, B., Zasońska, B. A., Stojadinović, S., and Ćirić-Marjanović, G., 2020, Novel Microporous Composites of MOF-5 and Polyaniline with High Specific Surface Area, *Synth. Met.*, 116348(262), 1-10.
- Boonchun, A. and Lambrecht, W.R., 2009, Bond Lengths, Phase Stability, And Band Gaps in Mg<sub>x</sub>Zn<sub>1-x</sub>O Alloys, *J. Vac. Sci. Technol. B*, 27(3), 1717-1721.
- Bordiga, S., Vitillo, J. G., Ricchiardi, G., Regli, L., Cocina, D., Zecchina, A., Arstad, B. Bjorgen, M., Hafizovic, J., and Lillerud, K. P., 2005, Interaction of Hydrogen with MOF-5, *J. Phys. Chem. B*, 109(39), 18237-18242.
- Broom, D.P., 2011, *Hydrogen Storage Materials: The Characterisation of Their Storage Properties*, Springer, London.

- Buda, C., and Dunietz, B.D., 2006, Hydrogen Physisorption on The Organic Linker in Metal Organic Frameworks: Ab Initio Computational Study, *J. Phys. Chem. B*, 110(21), 10479-10484.
- Campañá, C., Mussard, B., and Woo, T.K., 2009, Electrostatic Potential Derived Atomic Charges for Periodic Systems Using a Modified Error Functional, *J. Chem. Theory Comput.*, 5(10), 2866-2878.
- Carcassi, M.N. and Fineschi, F., 2005, Deflagrations of H<sub>2</sub> Air and CH<sub>4</sub> Air Lean Mixtures in A Vented Multi-Compartment Environment, *J. Energy*, 30(8), 1439-1451.
- Catão, A.J. L., and López-Castillo, A., 2017, Stability and Molecular Properties of The Boron-Nitrogen Alternating Analogs of Azulene and Naphthalene: A Computational Study, *J. Mol. Model.*, 23, 1-12.
- Chen, Y., Liu, M., Ma, Q., and Yang, M., 2022, Metal Organic Framework for Hydrogen Storage, *Highlights in Sci., Eng. and Technol.*, 6, 211-218.
- Crabtree, R.H., 2008, Hydrogen Storage in Liquid Organic Heterocycles, *Energy Environ. Sci.*, 1(1), 134-138.
- Dinca, M., Dailly, A., Liu, Y., Brown, C.M., Neumann, D.A., and Long, J.R., 2006, Hydrogen Storage in a Microporous Metal- Organic Framework with Exposed Mn<sup>2+</sup> Coordination Sites, *J. Am. Chem. Soc.*, 128(51), 16876-16883.
- Dubbeldam, D., Calero, S., Ellis, D. E., and Snurr, R. Q., 2015, RASPA: Molecular Simulation Software for Adsorption and Diffusion in Flexible Nanoporous Materials, *Mol. Simul.*, 42(2), 81-101.
- Eberle, U., Felderhoff, M., and Schüth, F., 2009, Chemical and Physical Solutions for Hydrogen Storage, *Angew. Chem. Int. Ed.*, 48(36), 6608-6630.
- Engelberts, J.J., Havenith, R.W., Van Lenthe, J.H., Jenneskens, L.W., and Fowler, P.W., 2005, The Electronic Structure of Inorganic Benzenes: Valence Bond and Ring-Current Descriptions, *Inorg. Chem.*, 44(15), 5266-5272.
- Frenkel, D., 2004, Introduction to Monte Carlo Methods, *NIC series*, 23, 29-60.
- Grimme, S., 1993, Ab Initio Study of the Structure and Dipole Moment of Azulene, *Chem. Phys. Lett.*, 201(1-4), 67-74.
- Grimme, S., Antony, J., Ehrlich, S., and Krieg, H., 2010, A Consistent and Accurate Ab Initio Parametrization of Density Functional Dispersion Correction (DFT-D) for The 94 Elements H-Pu, *J. Chem. Phys.* 132(15), 154104.
- Grochala, W., and Edwards, P.P., 2004, Thermal Decomposition of the Non-Interstitial Hydrides for The Storage and Production of Hydrogen, *Chem. Rev.*, 104(3), 1283-1316.

- Gümüş, S., 2013, A Computational Study on Azaazulenes, *Heterocycl. Commun.*, 19(5), 369-373.
- Gupta, R.B., 2008, *Hydrogen fuel: production, transport, and storage*, CRC press, New York.
- Hinchliffe, A. and Soscún, H.J., 2005, Ab Initio Studies of The Dipole Moment and Polarizability of Azulene in Its Ground and Excited Singlet States, *Chem. Phys. Lett.*, 412(4-6), 365-368.
- Hosseini, S.E. and Wahid, M.A., 2016, Hydrogen Production from Renewable and Sustainable Energy Resources: Promising Green Energy Carrier for Clean Development, *Renew. Sust. Energ. Rev.*, 57, 850-866.
- Huang, B. and Lee, H., 2012, Defect and Impurity Properties of Hexagonal Boron Nitride: A First-Principles Calculation, *Phys. Rev. B*, 86(24), 245406.
- Hübner, O., Glöss, A., Fichtner, M., and Kloppe, W., 2004, On The Interaction of Dihydrogen with Aromatic Systems, *J. Phys. Chem. A*, 108(15), 3019-3023.
- Hutter, J., Iannuzzi, M., Schiffmann, F., and VandeVondele, J., 2014, Cp2k: Atomistic Simulations of Condensed Matter Systems, *Wiley Interdiscip. Rev. Comput. Mol. Sci.*, 4, 15-25.
- Kassaoui, M.E., Lakhal, M., Benyoussef, A., El Kenz, A., and Loulidi, M., 2021, Effect of Zinc Substitution by Magnesium and Cadmium on Hydrogen Storage Properties of Connector-Metal-Organic Framework-5, *J. Alloys Compd.*, 874, 159902.
- Kim, D., Lee, T.B., Choi, S.B., Yoon, J. H., Kim, J., and Choi, S.H., 2006, A Density Functional Theory Study of A Series of Functionalized Metal-Organic Frameworks, *Chem. Phys. Lett.*, 420(1-3), 256-260.
- Kinraide, T.B. and Yermiyahu, U., 2007, A Scale of Metal Ion Binding Strengths Correlating with Ionic Charge, Pauling Electronegativity, Toxicity, and Other Physiological Effects, *J. Inorg. Biochem.*, 101(9), 1201-1213.
- Kojima, Y., 2019, Hydrogen Storage Materials for Hydrogen and Energy Carriers, *Int. J. Hydrogen Energy*, 44(33), 18179-18192.
- Kökçam-Demir, Ü., Goldman, A., Esrafil, L., Gharib, M., Morsali, A., Weingart, O., and Janiak, C., 2020, Coordinatively Unsaturated Metal Sites (Open Metal Sites) in Metal-Organic Frameworks: Design and Applications, *Chem. Soc. Rev.*, 49(9), 2751-2798.
- Kong, X.J. and Li, J.R., 2021, An Overview of Metal-Organic Frameworks for Green Chemical Engineering, *Eng.*, 7(8), 1115-1139.
- Kumar, S. and Kumar, T.D., 2020, Hydrogen Trapping Potential of Ca Decorated Metal-Graphyne Framework, *Energy*, 199, 117453.

- Kuno, M., 2011, *Introductory Nanoscience: Physical and Chemical Concepts*, CRC Press, New York.
- Langmi, H.W., Ren, J., North, B., Mathe, M., and Bessarabov, D., 2014, Hydrogen Storage in Metal-Organic Frameworks: A Review, *Electrochim. Acta*, 128, 368-392.
- Levesque, D., Gicquel, A., Darkrim, F. L., and Kayiran, S. B., 2002, Monte Carlo Simulations of Hydrogen Storage in Carbon Nanotubes, *J. Phys. Condens. Matter*, 14(40), 9285.
- Lewars, E., 2011, *Computational Chemistry. Introduction to The Theory and Applications of Molecular and Quantum Mechanics*, Springer, London.
- Li, H., Wang, K., Sun, Y., Lollar, C.T., Li, J., and Zhou, H.C., 2018, Recent Advances in Gas Storage and Separation Using Metal–Organic Frameworks, *Mater. Today*, 21(2), 108-121.
- Li, H., Wang, K., Sun, Y., Lollar, C.T., Li, J., and Zhou, H.C., 2018, Recent Advances in Gas Storage and Separation Using Metal–Organic Frameworks, *Mater. Today*, 21(2), 108-121.
- Liu, C., Li, F., Ma, L. P., and Cheng, H. M., 2010, Advanced Materials for Energy Storage, *Adv. Mater.*, 22(8), E28-E62.
- Liu, Y., Eubank, J.F., Cairns, A.J., Eckert, J., Kravtsov, V.C., Luebke, R., and Eddaoudi, M., 2007, Assembly of Metal–Organic Frameworks (MOFs) Based on Indium-Trimer Building Blocks: A Porous MOF with Soc Topology and High Hydrogen Storage, *Angew. Chem.*, 119(18), 3342-3347.
- Lotfi, R., and Saboohi, Y., 2014, Effect of Metal Doping, Boron Substitution and Functional Groups on Hydrogen Adsorption of MOF-5: A DFT-D Study, *Comput. Theor. Chem.*, 1044, 36-43.
- Manoharan, Y., Hosseini, S.E., Butler, B., Alzahrani, H., Senior, B.T.F., Ashuri, T., and Krohn, J., 2019, Hydrogen Fuel Cell Vehicles; Current Status and Future Prospect, *Appl. Sci.*, 9(11), 2296.
- Manz, T.A., and Limas, N.G., 2016. Introducing DDEC6 Atomic Population Analysis: Part 1. Charge Partitioning Theory and Methodology, *RSC Adv.*, 6, 47771–47801.
- Martinez-Guajardo, G., Donald, K.J., Wittmaack, B.K., Vazquez, M.A., and Merino, G., 2010, Shorter Still: Compressing C-C Single Bonds, *Org. Lett.*, 18 (12), 4058-4061.
- Mayo, S.L., Olafson, B.D., and Goddard, W.A., 1990, DREIDING: A Generic Force Field for Molecular Simulations, *J. Phys. Chem.*, 94(26), 8897–8909.
- Möllerstedt, H., Piqueras, M.C., Crespo, R., and Ottosson, H., 2004, Fulvenes, Fulvalenes, and Azulene: Are They Aromatic Chameleons?, *J. Am. Chem. Soc.*, 126(43), 13938-13939.

- Mulliken, R.S., 1955, Electronic Population Analysis on LCAO–MO Molecular Wave Functions, *I. J. Chem. Phys.*, 23, 1833–1840.
- Murray, L. J., Dincă, M., and Long, J.R., 2009, Hydrogen Storage in Metal–Organic Frameworks, *Chem. Soc. Rev.*, 38(5), 1294–1314.
- Neese, F., Wennmohs, F., Becker, U., and Riplinger, C., 2020, The ORCA Quantum Chemistry Program Package, *J. Phys. Chem.*, 152(22), 224108.
- Nelson Jr, R.D., Lide Jr, D.R., and Maryott, A.A., 1967, *Selected Values of Electric Dipole Moments for Molecules in The Gas Phase*, National Standard Reference Data System.
- Nguyen-Thuy, T., Le-Hoang, P., Vu, N.H., Le, T.N., Doan, T.L.H., Kuo, J., Nguyen, T.T., Pha, T.B., and Nguyen-Manh, D., 2020, Hydrogen Adsorption Mechanism of MOF-74 Metal–Organic Frameworks: An Insight from First Principles Calculations, *RSC Adv.*, 10(72), 43940 – 43949.
- Olabi, A.G., and Abdelkareem, M.A., 2022, Renewable Energy and Climate Change, *Renewable and Sustainable Energy Rev.*, 112111(158), 1–7.
- Perdew, J.P., Ruzsinszky, A., Csonka, G.I., Vydrov, O.A., Scuseria, G.E., Constantin, L.A., Zhou, X., and Burke, K., 2008, Restoring The Density-Gradient Expansion for Exchange in Solids and Surfaces, *Phys. Rev. Lett.*, 100, 1–4.
- Piaccenza, M. and Grimme, S., 2005, Van Der Waals Complexes of Polar Aromatic Molecules: Unexpected Structures for Dimers of Azulene, *J. Am. Chem. Soc.*, 127(42), 14841–14848.
- Prasetyo, N., and Pambudi, F.I., 2021, Toward Hydrogen Storage Material in Fluorinated Zirconium Metal–Organic Framework (MOF-801): A Periodic Density Functional Theory (DFT) Study of Fluorination and Adsorption, *Int. J. Hydrogen Energy*, 46(5), 4222–4228.
- Radenković, S., Marković, S., and Milenković, V., 2012, Electronic Structure Study of the Triplet Azulene-Like Molecules, *Chem. Phys. Lett.*, 545, 132–137.
- Ree, N., Andersen, C.L., Kilde, M.D., Hammerich, O., Nielsen, M.B., and Mikkelsen, K.V., 2018, The Quest for Determining One-Electron Redox Potentials of Azulene-1-Carbonitriles by Calculation, *Phys. Chem. Chem. Phys.*, 20(11), 7438–7446.
- Ren, J., Musyoka, N.M., Langmi, H.W., North, B.C., Mathe, M., Kang, X., and Liao, S., 2015, Hydrogen Storage in Zr-Fumarate MOF, *Int. J. Hydrogen Energy*, 40(33), 10542–10546.
- Rowsell, J.L., and Yaghi, O.M., 2005, Strategies for Hydrogen Storage in Metal–Organic Frameworks, *Angew. Chem. Int. Ed.*, 44(30), 4670–4679.
- Sava, D.F., Kravtsov, V.C., Nouar, F., Wojtas, L., Eubank, J.F., and Eddaoudi, M., 2008, Quest for Zeolite-Like Metal–Organic Frameworks: on



- Pyrimidinecarboxylate Bis-Chelating Bridging Ligands, *J. Am. Chem. Soc.*, 130(12), 3768-3770.
- Schlapbach, L. and Züttel, A., 2001, Hydrogen-Storage Materials for Mobile Applications, *Nature*, 414(6861), 353-358.
- Senkov, O.N., and Scott, J.M., 2004, Formation and Thermal Stability of Ca–Mg–Zn and Ca–Mg–Zn–Cu Bulk Metallic Glasses, *Mater. Lett.*, 58(7-8), 1375-1378.
- Sherif, S.A., Zeytinoglu, N., and Veziroğlu, T.N., 1997, Liquid Hydrogen: Potential, Problems, and a Proposed Research Program, *Int. J. Hydrogen Energy*, 22(7), 683–688.
- Shet, S. P., Priya, S. S., Sudhakar, K., and Tahir, M., 2021, A Review on Current Trends in Potential Use of Metal-Organic Framework for Hydrogen Storage, *Int. J. Hydrogen Energy*, 46(21), 11782-11803.
- Suksaengrat, P., Amornkitbamrung, V., Srepusharawoot, P., and Ahuja, R., 2016, Density Functional Theory Study of Hydrogen Adsorption in a Ti-Decorated Mg-Based Metal–Organic Framework-74, *ChemPhysChem*, 17(6), 879-884.
- Sutapa, I.W., Armunanto, R., and Wijaya, K., 2010, Effect of Scandium on Hydrogen Dissociation Energy at Magnesium Surface: Ab Initio DFT Study, *Indones. J. Chem.* 10, 184–188.
- Vitillo, J.G., Regli, L., Chavan, S., Ricchiardi, G., Spoto, G., Dietzel, P.D., Bordiga, S., and Zecchina, A., 2008, Role of Exposed Metal Sites in Hydrogen Storage in Mofs, *J. Am. Chem. Soc.*, 130(26), 8386-8396.
- Von Helmolt, R. and Eberle, U., 2007, Fuel Cell Vehicles: Status 2007, *J. Power Sources*. 165, 833–843.
- Wang, P. and Kang, X.D., 2008, Hydrogen-Rich Boron-Containing Materials for Hydrogen Storage, *Dalton Trans.*, 5400–5413.
- Wang, Y., Lan, Z., Huang, X., Liu, H., and Guo, J., 2019, Study on Catalytic Effect and Mechanism of MOF (MOF = ZIF-8, ZIF-67, MOF-74) on Hydrogen Storage Properties of Magnesium, *Int. J. Hydrogen Energy*, 44(54), 28863-28873.
- Wong, M., Van Kuiken, B.E., Buda, C., and Dunietz, B.D., 2009, Multiadsorption and Coadsorption of Hydrogen on Model Conjugated Systems, *J. Phys. Chem. C*, 113(28), 12571-12579.
- Wong, M., Van-Kuiken, B.E., Buda, C., and Dunietz, B.D., 2009, Multiadsorption and Coadsorption of Hydrogen on Model Conjugated Systems, *J. Phys. Chem. B C*, 113(28), 12571-12579.
- Xia, L. and Liu, Q., 2017, Adsorption of H<sub>2</sub> on Aluminum-Based Metal-Organic Frameworks: A Computational Study, *Comput. Mat. Sci.*, 126, 176-181.

- Xia, L., and Wang, F., 2016, Prediction of Hydrogen Storage Properties of Zr-Based Mofs, *Inorg. Chim. Acta*, 444, 186-192.
- Xin, H., Li, J., Yang, X., and Gao, X., 2019, Azulene-Based BN-Heteroaromatics, *J. Org. Chem.*, 85(1), 70-78.
- Yu, S., Jing, G., Li, S., Li, Z., and Ju, X., 2020, Tuning The Hydrogen Storage Properties of MOF-650: a Combined DFT and GCMC Simulations Study, *Int. J. Hydrogen Energy*, 45(11), 6757-6764.
- Yu, S., Li, S., Meng, X., Wan, C., and Ju, X., 2018, Tuning The Hydrogen Adsorption Properties of Zn-Based Metal–Organic Frameworks: Combined DFT and GCMC Simulations, *J. Solid State Chem.*, 266, 31-36.
- Zhang, J., and Lu, T., 2021, Efficient Evaluation of Electrostatic Potential with Computerized Optimized Code, *Phys. Chem. Chem. Phys.*, 23(36), 20323-20328.