

DAFTAR PUSTAKA

- Abednatanzi, S., Derakhshandeh, P.G., Depauw, H., Coudert, F., Vrielinck, H., Voort, P.V.D., Leus, K., 2019, Mixed-Metal Metal–Organic Frameworks, *Chem. Soc. Rev.*, 48(9), 2535–2565.
- An, Y., Lv, X., Jiang, W., Wang, L., Shi, Y., Hang, X., Pang, H., 2024, The Stability of MOFs in Aqueous Solutions—Research Progress and Prospects, *Green Chem. Eng.*, 5(2), 187-204.
- Botas, J.A., Calleja, G., Sánchez-Sánchez, M., Orcajo, M.G. 2011, Effect of Zn/Co ratio in MOF-74 Type Materials Containing Exposed Metal Sites on Their Hydrogen Adsorption Behaviour and on Their Band Gap Energy, *Int. J. Hydrogen Energy*, 36(17), 10834-10844.
- Byrd, R.H., Lu, P., Nocedal, J., Zhu, C., A Limited Memory Algorithm for Bound Constrained Optimization, *SIAM J SCI COMPUT*, 16(5), 1190-1208.
- Choe, J.H., Kim, H., Hong, C.S., 2021, MOF-74 Type Variants for CO₂ Capture, *Mater. Chem. Front.*, 5(14), 5172-5185.
- Chung, Y.G., Haldoupis, E., Bucior, B.J., Haranczyk, M., Lee, S., Zhang, H., Vogiatzis, K.D., Milisavljevic, M., Ling, S., Camp, J.S., Slater, B., Siepmann, J.I., Sholl, D.S., Snurr, R.Q., 2019, Advances, Updates, and Analytics for the Computation-Ready, Experimental Metal–Organic Framework Database: CoRE MOF 2019, *J. Chem. Eng. Data*, 64(12), 5985–5998.
- Cohen, S.M., Rosi, N.L., 2021, Postsynthetic Modification of Metal–Organic Frameworks, *Inorg. Chem.*, 60(16), 11703–11705.
- D’Alessandro, D.M., Smit, B., Long, J.R., 2010, Carbon Dioxide Capture: Prospects for New Materials, *Angew. Chem. Int. Ed.*, 49, 6058-6082.
- Ebrahim, A.M., Bandosz, T.J., 2013, Ce(III) Doped Zr-Based MOFs as Excellent NO₂ Adsorbents at Ambient Conditions, *ACS Appl. Mater. Interfaces*, 5(21), 10565–10573.
- Eddaoudi, M., Kim, J., Rosi, N., Vodak, D., Wachter, J., O’Keeffe, M., Yaghi, O.M., 2002, Systematic Design of Pore Size and Functionality in Isorecticular MOFs and Their Application in Methane Storage, *Science*, 295(5554), 469-472.
- Goedecker, S., Teter, M., Hutter, J., 1996, Separable Dual-space Gaussian Pseudopotentials, *Phys. Rev. B*, 54(3), 1703-1710.

- Gopalsamy, K., Wahiduzzaman, M., Daouli, A., Badawi, M., Maurin, G., 2022, Computational Exploration of a Metal(II) Catecholate-Functionalized UiO-66 Nanoporous Metal–Organic Framework for Effective NO_x Capture, *ACS Appl. Nano Mater.*, 5(10), 15123–15132.
- Grimme, S., Antony, J., Ehrlich, S., 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.
- Guidon, M., Hutter, J., VandeVondele, J., 2010, Auxiliary Density Matrix Methods for Hartree-Fock Exchange Calculations, *J. Chem. Theory Comput.*, 6(8), 2348–2364.
- Hall, J.N., Bollini, P., 2020, Quantification of Open-Metal Sites in Metal–Organic Frameworks Using Irreversible Water Adsorption, *Langmuir*, 36(5), 1345–1356.
- Hofmann, D.J., Butler, J.H., Tans, P.P., 2009, A New Look at Atmospheric Carbon Dioxide, *Atmos. Environ.*, 43 (12), 2084–2086.
- Howe, J.D., Morelock, C.R., Jiao, Y., Chapman, K.W., Walton, K.S., Sholl, D.S., 2017, Understanding Structure, Metal Distribution, and Water Adsorption in Mixed-Metal MOF-74, *J. Phys. Chem. C*, 121(1), 627–635.
- Hu, H., Xu, K., 2020, *Physicochemical Technologies for HRP and Risk Control*, In Ren, H., Zhang, X., *High-Risk Pollutants in Wastewater*, Elsevier, Amsterdam.
- Islamoglu, T., Chen, Z., Wasson, M.C., Buru, C.T., Kirlikovali, K.O., Afrin, U., Mian, M.R., Farha, O.K., 2020, Metal–Organic Frameworks Against Toxic Chemicals, *Chem. Rev.*, 120(16), 8130–8160.
- Jaryal, R., Kumar, R., Khullar, S., 2022, Mixed Metal-Metal Organic Frameworks (MM-MOFs) and Their Use as Efficient Photocatalysts for Hydrogen Evolution from Water Splitting Reactions, *Coord. Chem. Rev.*, 464, 214542.
- Jiao, Y., Morelock, C.R., Burtch, N.C., Mounfield III, W.P., Hungerford, J.T., Walton, K.S., 2015, Tuning the Kinetic Water Stability and Adsorption Interactions of Mg-MOF-74 by Partial Substitution with Co or Ni, *Ind. Eng. Chem. Res.*, 54(49), 12408–12414.
- Kim, D., Coskun, A., 2017, Template-Directed Approach Towards the Realization of Ordered Heterogeneity in Bimetallic Metal–Organic Frameworks, *Angew. Chem. Int. Ed.*, 56(18), 5071–5076.
- Kizzie, A.C., Wong-Foy, A.G., Matzger, A.J., 2011, Effect of Humidity on the Performance of Microporous Coordination Polymers as Adsorbents for CO₂ Capture, *Langmuir*, 27(10), 6368–6373.

- Kühne, T.D., Iannuzzi, M., Ben, M.D., Rybkin, V.V., Seewald, P., Stein, F., Laino, T., Khaliullin, R.Z., Schütt, O., Schiffmann, F., Golze, D., Wilhelm, J., Chulkov, S., Bani-Hashemian, M.H., Weber, V., Borštnik, U., Taillefumier, M., Jakobovits, A.S., Lazzaro, A., Pabst, H., Müller, T., Schade, R., Guidon, M., Andermatt, S., Holmberg, N., Schenter, G.K., Hehn, A., Bussy, A., Belleflamme, F., Tabacchi, G., Glöß, A., Lass, M., Bethune, I., Mundy, C.J., Plessl, C., Watkins, M., VandeVondele, J., Krack, M., Hutter, J., 2020, CP2K: An Electronic Structure and Molecular Dynamics Software Package - Quickstep: Efficient and Accurate Electronic Structure Calculations, *J. Chem. Phys.*, 152(19), 194103.
- Lee, K., Howe, J.D., Lin, L., Smit, B., Neaton, J.B., 2015, Small-Molecule Adsorption in Open-Site Metal–Organic Frameworks: A Systematic Density Functional Theory Study for Rational Design, *Chem. Mater.*, 27(3), 668–678.
- Li, B., Wen, H., Zhou, W., Chen, B., 2014, Porous Metal–Organic Frameworks for Gas Storage and Separation: What, How, and Why?, *J. Phys. Chem. Lett.*, 5(20), 3468-3479.
- Li, D., Li, N., Liu, W., Xu, S., Sun, Y., Qiao, Z., Zhong, C., 2023, Highly Water-stable MOF-74 Synthesized by *in-situ* Trace Polymer Modification, *Polymer*, 281, 126112.
- Li, Y., Wang, X., Xu, D., Chung, J.D., Kaviani, M., Huang, B., 2015, H₂O Adsorption/Desorption in MOF-74: *Ab Initio* Molecular Dynamics and Experiments, *J. Phys. Chem. C*, 119(23), 13021–13031.
- Liu, J., Pan, Y., 2020, *Mixed-metal Systems for the Synthesis of MOFs*, In Mozafari, M., *Metal-Organic Frameworks for Biomedical Applications*, Elsevier, Amsterdam.
- Lu, T., Chen, F., 2012, Multiwfn: A multifunctional Wavefunction Analyzer, *J. Comput. Chem.*, 33(5), 580-592.
- Mahajan, S., Lahtinen, M., 2022, Recent Progress in Metal-Organic Frameworks (MOFs) for CO₂ capture at different pressures, *J. Environ. Chem. Eng.*, 10(6), 108930.
- Marti, R.M., Howe, J.D., Morelock, C.R., Conradi, M.S., Walton, K.S., Sholl, D.S., Hayes, S.E., 2017, CO₂ Dynamics in Pure and Mixed-Metal MOFs with Open Metal Sites, *J. Phys. Chem. C*, 121(46), 25778–25787.
- Masoomi, M.Y., Morsali, A., Dhakshinamoorthy, A., Garcia, H., 2019, Mixed-Metal MOFs: Unique Opportunities in Metal-organic Framework Functionality and Design, *Angew. Chem. Int. Ed.*, 58(43), 15188-15205.

- Millward, A.R., Yaghi, O.M., Metal-Organic Frameworks with Exceptionally High Capacity for Storage of Carbon Dioxide at Room Temperature, *J. Am. Chem. Soc.*, 127(51), 17998–17999.
- Momma, K., Izumi, F., 2008, VESTA: A Three-Dimensional Visualization System for Electronic and Structural Analysis, *J. Appl. Crystallogr.*, 41(3), 653–658.
- Nguyen, V.T.T., Luu, C.L., Nguyen, T., Nguyen, A.P., Hoang, C.T., Ha, A.C., 2020, Multifunctional Zn-MOF-74 as the Gas Adsorbent and Photocatalyst, *Adv. Nat. Sci.: Nanosci. Nanotechnol.*, 11(3), 35008.
- Orio, M., Pantazis, D.A., Neese, F., 2009, Density Functional Theory, *Photosynth Res*, 102, 443–453.
- Oliveira, A.D., Lima, G.F.D., Abreu, H.A.D., 2018, Structural and Electronic Properties of M-MOF-74 (M=Mg, Co or Mn), *Chem. Phys. Lett.*, 691, 283–290.
- Pambudi, F.I., 2022, Electronic Properties of Heterometallic Zeolitic Imidazolate Framework and Its Encapsulation with Ni, Pd and Pt, *Inorg. Chem. Commun.*, 143, 109798.
- Pambudi, F.I., Prasetyo, N., 2022, Theoretical Investigation on The Structure of Mixed-metal Zeolitic Imidazolate Framework and Its Interaction with CO₂, *Comput. Mater. Sci.*, 210, 111033.
- Perdew, J.P., Burke, K., Ernzerhof, M., 1996, Generalized Gradient Approximation Made Simple, *Phys. Rev. Lett.*, 77(18), 3865–3868.
- Priandani, L., Aliefa, A., Arjasa, O.P., Pambudi, F.I., 2023, An Experimental and Computational Study of Zeolitic Imidazole Framework (ZIF-8) Synthesis Modulated with Sodium Chloride and Its Interaction with CO₂, *Bull. Chem. React. Eng.*, 18(3), 521–538.
- Skalska, K., Miller, J.S., Ledakowicz, S., 2010, Trends in NO_x Abatement: A Review, *Sci. Total Environ.*, 408(19), 3976–3989.
- Tan, K., Zuluaga, S., Wang, H., Canepa, P., Soliman, K., Cure, J., Li, J., Thonhauser, T., Chabal, Y.J., 2017, Interaction of Acid Gases SO₂ and NO₂ with Coordinatively Unsaturated Metal Organic Frameworks: M-MOF-74 (M = Zn, Mg, Ni, Co), *Chem. Mater.*, 29(10), 4227–4235.
- Tan, K., Ullah, S., Pandey, H., Cedeño-Morales, E.M., Wang, H., Wang, K., Zhou, H., Li, J., Thonhauser, T., 2022, Competitive Adsorption of NH₃ and H₂O in Metal–Organic Framework Materials: MOF-74, *Chem. Mater.*, 34(17), 7906–7915.
- Tien, C., 2018, *Introduction to Adsorption: Basics, Analysis, and Applications*, Elsevier, Amsterdam.

- Vallenzano, L., Civalleri, B., Chavan, S., Palomino, G.T., Arean, C.O., Bordiga, S., 2010, Computational and Experimental Studies on the Adsorption of CO, N₂, and CO₂ on Mg-MOF-74, *J. Phys. Chem. C*, 114(25), 11185–11191.
- VandeVondele, J., Hutter, J., 2007, Gaussian Basis Sets for Accurate Calculations on Molecular Systems in Gas and Condensed Phases, *J. Chem. Phys.*, 127(11), 114105.
- Villajos, J.A., Jagorel, N., Reinsch, S., Emmerling, F., 2019, Increasing Exposed Metal Site Accessibility in a Co-MOF-74 Material With Induced Structure-Defects, *Front. Mater.*, 6.
- Xiao, T., Liu, D., 2019, The Most Advanced Synthesis and a Wide Range of Applications of MOF-74 and Its Derivatives, *Microporous Mesoporous Mater.*, 283, 88-103.
- Yazaydin, A.Ö., Snurr, R.Q., Park, T., Koh, K., Liu, J., LeVan, M.D., Benin, A.I., Jakubczak, P., Lanuza, M., Galloway, D.B., Low, J.J., Willis, R.R., 2009, Screening of Metal-Organic Frameworks for Carbon Dioxide Capture from Flue Gas Using a Combined Experimental and Modeling Approach, *J. Am. Chem. Soc.*, 131(51), 18198-18199.
- Yu, J., Xie, L., Li, J., Ma, Y., Seminario, J.M., Balbuena, P.B., 2017, CO₂ Capture and Separations Using MOFs: Computational and Experimental Studies, *Chem. Rev.*, 117(14), 9674–9754.
- Yu, S., Jing, G., Li, S., Li, Z., Ju, X., 2020, Tuning The Hydrogen Storage Properties of MOF-650: A Combined DFT and GCMC Simulations Study, *Int. J. Hydrog. Energy.*, 45(11), 6757-6764.
- Yusuf, V.F., Malek, N.I., Kailasa, S.K., 2022, Review on Metal–Organic Framework Classification, Synthetic Approaches, and Influencing Factors: Applications in Energy, Drug Delivery, and Wastewater Treatment, *ACS Omega*, 7(49), 44507–44531.
- Zafar, F., Sharmin, E., 2016, *Metal-Organic Frameworks*, Books on Demand, Norderstedt.
- Zhao, M., Yang, Y., Gu, X., 2023, MOF based CO₂ capture: Adsorption and Membrane Separation, *Inorg. Chem. Commun.*, 152, 110722.