Lignin-related computational chemistry literature

- Reviews: [1, 2, 3, 3, 4]
- Quantum mechanics: [5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22]
- Force field development: [23, 24]
- Molecular dynamics: [25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 19]
- ReaxFF: [36]
- Coarse-grained: [37]

References

[1] Loukas Petridis, Sai Venkatesh Pingali, Volker Urban, William T. Heller, Hugh M. O'Neill, Marcus Foston, Arthur Ragauskas, and Jeremy C. Smith. Self-similar multiscale structure of lignin revealed by neutron scattering and molecular dynamics simulation. *Physical Review E*, 83(6), jun 2011.

[2] Amandeep K. Sangha, Loukas Petridis, Jeremy C. Smith, Angela Ziebell, and Jerry M. Parks. Molecular simulation as a tool for studying lignin. *Environmental Progress & Sustainable Energy*, 31(1):47–54, dec 2011.

[3] J. D. Murillo, J. J. Biernacki, S. Northrup, and A. S. Mohammad. Biomass pyrolysis kinetics: A review of molecular-scale modeling contributions. *Brazilian Journal of Chemical Engineering*, 34(1):1–18, jan 2017.

[4] Yaqin Zhang, Hongyan He, Yanrong Liu, Yanlei Wang, Feng Huo, Maohong Fan, Hertanto Adidharma, Xuehui Li, and Suojiang Zhang. Recent progress in theoretical and computational studies on the utilization of lignocellulosic materials. *Green Chemistry*, 21(1):9–35, 2019.

[5] K. L. Mardis, A. J. Glemza, B. J. Brune, G. F. Payne, and M. K. Gilson. Differential adsorption of phenol derivatives onto a polymeric sorbent: a combined molecular modeling and experimental study. *The Journal of Physical Chemistry B*, 103(45):9879–9887, nov 1999.

[6] B. Durbeej and L.A. Eriksson. A density functional theory study of coniferyl alcohol intermonomeric cross linkages in lignin - three-dimensional structures, stabilities and the thermodynamic control hypothesis. *Holzforschung*, 57(2), jan 2003.

[7] B. Durbeej and L. A. Eriksson. Formation of β-o-4 lignin models -a theoretical study. *Holzforschung*, 57(5), jan 2003.

[8] Ariana Beste and A. C. Buchanan. Computational study of bond dissociation enthalpies for lignin model compounds. substituent effects in phenethyl phenyl ethers. *The Journal of Organic Chemistry*, 74(7):2837–2841, apr 2009.

[9] Yi ru Chen and Simo Sarkanen. Macromolecular replication during lignin biosynthesis. *Phytochemistry*, 71(4):453–462, mar 2010.

[10] Mark W. Jarvis, John W. Daily, Hans-Heinrich Carstensen, Anthony M. Dean, Shantanu Sharma, David C. Dayton, David J. Robichaud, and Mark R. Nimlos. Direct detection of products from the pyrolysis of 2-phenethyl phenyl ether. *The Journal of Physical Chemistry A*, 115(4):428–438, feb 2011.

[11] Seonah Kim, Stephen C. Chmely, Mark R. Nimlos, Yannick J. Bomble, Thomas D. Foust, Robert S. Paton, and Gregg T. Beckham. Computational study of bond dissociation enthalpies for a large range of native and modified lignins. *The Journal of Physical Chemistry Letters*, 2(22):2846–2852, oct 2011.

[12] Chirantha P. Rodrigo, William H. James, and Timothy S. Zwier. Single-conformation ultraviolet and infrared spectra of jet-cooled monolignols:p-coumaryl alcohol, coniferyl alcohol, and sinapyl alcohol. *Journal of the American Chemical Society*, 133(8):2632–2641, mar 2011.

[13] Heath D. Watts, Mohamed Naseer Ali Mohamed, and James D. Kubicki. Evaluation of potential reaction mechanisms leading to the formation of coniferyl alcohol α-linkages in lignin: a density functional theory study. *Physical Chemistry Chemical Physics*, 13(47):20974, 2011.

[14] Wu Qin, Lingnan Wu, Zongming Zheng, Changqing Dong, and Yongping Yang. Lignin hydrolysis and phosphorylation mechanism during phosphoric acid–acetone pretreatment: A DFT study. *Molecules*, 19(12):21335–21349, dec 2014.

[15] Jinbao Huang, Chao He, Chao Liu, Hong Tong, Longqin Wu, and Shubin Wu. A computational study on thermal decomposition mechanism of β-1 linkage lignin dimer. *Computational and Theoretical Chemistry*, 1054:80–87, feb 2015.

[16] Jinbao Huang and Chao He. Pyrolysis mechanism of α-o-4 linkage lignin dimer: A theoretical study. *Journal of Analytical and Applied Pyrolysis*, 113:655–664, may 2015.

[17] Lei Chen, Xiaoning Ye, Feixian Luo, Jingai Shao, Qiang Lu, Yang Fang, Xianhua Wang, and Hanping Chen. Pyrolysis mechanism of β o 4 type lignin model dimer. *Journal of Analytical and Applied Pyrolysis*, 115:103–111, sep 2015.

[18] Thomas Elder and Raymond C Fort Jr. Reactivity of lignin—correlation with molecular orbital calculations. In Cyril Heitner, Donald R Dimmel, and John A Schmidt, editors, *Lignin and lignans: Advances in chemistry*, pages 321–347. CRC Press, Taylor & Francis Group, Boca Raton, FL, 2016.

[19] Zhang Junjiao, Zhu Jinqi, Lin Changfeng, Wang Tipeng, Dong Changqing, and Qin Wu. Pretreatment mechanism of β-o-4 lignin during phosphoric acid-acetone process based on density functional theory and molecular dynamic simulations. *International Journal of Agricultural and Biological Engineering*, 9(2):127–136, 2016.

[20] Ángel Sánchez-González, Francisco J. Martín-Martínez, and J. A. Dobado. The role of weak interactions in lignin polymerization. *Journal of Molecular Modeling*, 23(3):80, Feb 2017.

[21] Yaqin Zhang, Hongyan He, Kun Dong, Maohong Fan, and Suojiang Zhang. A DFT study on lignin dissolution in imidazolium-based ionic liquids. *RSC Advances*, 7(21):12670–12681, 2017.

[22] Terry Gani, Michael Orella, Eric Anderson, Michael Stone, Fikile Brushett, Gregg Beckham, and Yuriy Román-Leshkov. Quantum Mechanical Calculations Suggest That Lignin Polymerization Is Kinetically Controlled. 11 2018.

[23] Loukas Petridis and Jeremy C. Smith. A molecular mechanics force field for lignin. *Journal of Computational Chemistry*, 30(3):457–467, feb 2009.

[24] Josh V. Vermaas, Loukas Petridis, John Ralph, Michael F. Crowley, and Gregg T. Beckham. Systematic parameterization of lignin for the CHARMM force field. *Green Chemistry*, 21(1):109–122, 2019.

[25] Stéphane Besombes and Karim Mazeau. The cellulose/lignin assembly assessed by molecular modeling. part 1: adsorption of a threo guaiacyl β-o-4 dimer onto a iβ cellulose whisker. *Plant Physiology and Biochemistry*, 43(3):299–308, March 2005.

[26] Xiao Yi Li and Leif A. Eriksson. Molecular dynamics study of lignin constituents in water. *Holzforschung*, 59(3), jan 2005.

[27] Stéphane Besombes and Karim Mazeau. The cellulose/lignin assembly assessed by molecular modeling. part 2: seeking for evidence of organization of lignin molecules at the interface with cellulose. *Plant Physiology and Biochemistry*, 43(3):277–286, mar 2005.

[28] Loukas Petridis, Roland Schulz, and Jeremy C. Smith. Simulation analysis of the temperature dependence of lignin structure and dynamics. *Journal of the American Chemical Society*, 133(50):20277–20287, dec 2011.

[29] Landry Charlier and Karim Mazeau. Molecular modeling of the structural and dynamical properties of secondary plant cell walls: Influence of lignin chemistry. *The Journal of Physical Chemistry B*, 116(14):4163–4174, apr 2012.

[30] Eduardo W. Castilho-Almeida, Wagner B. De Almeida, and Hélio F. Dos Santos. Conformational analysis of lignin models: a chemometric approach. *Journal of Molecular Modeling*, 19(5):2149–2163, May 2013.

[31] Benjamin Lindner, Loukas Petridis, Roland Schulz, and Jeremy C. Smith. Solvent-driven preferential association of lignin with regions of crystalline cellulose in molecular dynamics simulation. *Biomacromolecules*, 14(10):3390–3398, sep 2013.

[32] Paul Langan, Loukas Petridis, Hugh M. O'Neill, Sai Venkatesh Pingali, Marcus Foston, Yoshiharu Nishiyama, Roland Schulz, Benjamin Lindner,

B. Leif Hanson, Shane Harton, William T. Heller, Volker Urban, Barbara R. Evans, S. Gnanakaran, Arthur J. Ragauskas, Jeremy C. Smith, and Brian H. Davison. Common processes drive the thermochemical pretreatment of lignocellulosic biomass. *Green Chem.*, 16(1):63–68, 2014.

[33] Wenzhuo Li, Jianlong Wang, Dingjia Xu, and Song Zhang. Study on adsorption and desorption of urea in lignosulfonate with molecular simulations. *Computational and Theoretical Chemistry*, 1033:60–66, apr 2014.

[34] Josh V. Vermaas, Loukas Petridis, Xianghong Qi, Roland Schulz, Benjamin Lindner, and Jeremy. C. Smith. Mechanism of lignin inhibition of enzymatic biomass deconstruction. *Biotechnology for Biofuels*, 8(1), dec 2015.

[35] Loukas Petridis and Jeremy C. Smith. Conformations of low-molecular-weight lignin polymers in water. *ChemSusChem*, 9(3):289–295, jan 2016.

[36] Ariana Beste. ReaxFF study of the oxidation of lignin model compounds for the most common linkages in softwood in view of carbon fiber production. *The Journal of Physical Chemistry A*, 118(5):803–814, jan 2014.

[37] Wenzhuo Li, Yingying Zhao, Shuaiyu Huang, Song Zhang, and Lin Zhang. Development and evaluation of an automatically adjusting coarse-grained force field for aβ-o-4 type lignin from atomistic simulations. *Modelling and Simulation in Materials Science and Engineering*, 25(1):015001, nov 2016.