2.9 References

(1) Yun, L.; Zhao, J.; Tang, X.; Ma, C.; Yu, Z.; Meng, Q. Selective Oxidation of Benzylic Sp^3C-H Bonds Using Molecular Oxygen in a Continuous-Flow Microreactor. *Org. Process Res. Dev.* **2021**, 25, 1612–1618.

(2) A. Arndtsen, B.; G. Bergman, R.; Andrew Mobley, T.; H. Peterson, T. Selective Intermolecular Carbon-Hydrogen Bond Activation by Synthetic Metal Complexes in Homogeneous Solution. *Acc. Chem. Res.* **2002**, *28*, 154–162.

(3) Sharma, A. S.; Kaur, H. Sustainable Protocol for Benzylic -CH_2 Oxidation with Dioxygen to Phenones Using AuNPs@ Resin Beads. *ChemistrySelect* **2017**, *2*, 10112–10117.

(4) Jones, W. D. The Effects of Ancillary Ligands on Metal–Carbon Bond Strengths as Determined by C–H Activation. *Top Organomet Chem* **2016**, *56*, 67–90.

(5) Wang, Y.; Wang, Y.; Kuang, Y. Rh2(Esp)2-Catalyzed Allylic and Benzylic Oxidations. *Chem. Commun.* **2015**, 51, 5852–5855.

(6) Zhang, J.; Wang, Z.; Wang, Y.; Wan, C.; Zheng, X.; Wang, Z. A Metal-Free Catalytic System for the Oxidation of Benzylic Methylenes and Primary Amines under Solvent-Free Conditions. *Green Chem.* **2009**, *11*, 1973–1978.

(7) Hruszkewycz, D. P.; Miles, K. C.; Thiel, O. R.; Stahl, S. S. Co/NHPI-Mediated Aerobic Oxygenation of Benzylic C-H Bonds in Pharmaceutically Relevant Molecules. *Chemi. Sci.* **2017**, *8*, 1282–1287.

(8) Yi, H.; Bian, C.; Hu, X.; Niu, L.; Lei, A. Visible Light Mediated Efficient Oxidative Benzylic Sp^3 C-H to Ketone Derivatives Obtained under Mild Conditions Using O_2. *Chem.l Commun.* **2015**, *51*, 14046–14049.

(9) Bai, Y.; Yang, T.; Gu, Q.; Cheng, G.; Zheng, R. Shape Control Mechanism of Cuprous Oxide Nanoparticles in Aqueous Colloidal Solutions. *Powder Technol.* **2012**, *227*, 35–42.

(10) K. Machhi, H.; K. Sonigara, K.; N. Bariya, S.; P. Soni, H.; S. Soni, S. Hierarchically Porous Metal–Organic Gel Hosting Catholyte for Limiting Iodine Diffusion and Self-Discharge Control in Sustainable Aqueous Zinc–I_2 Batteries. *ACS Appl. Mater. Interfaces* **2021**, *13*, 21426–21435.

(11) P. Giannozzia, O. Andreussib,i, T. Brummec, O. Bunaud, M. Buongiorno Nardellie, M. Calandrad, R. Carf, C. Cavazzonig, D. Ceresolih, M. C. et al. Advanced Capabilities for Materials Modelling with Quantum ESPRESSO. *Mater. Res. Express* **2019**, 0–12.

(12) Stefan Grimme, Stephan Ehrlich, L. G. Effect of the Damping Function in Dispersion Corrected Density Functional Theory . *J. Comput. Chem*. **2012**, *32*, 174–182.

(13) Hendrik J. Monkhorst and James D. Pack. Special Points for Brillonin-Zone Integrations. *Paper Knowledge . Toward a Media History of Documents* **2014**, *13*, 5188–5192.

(14) Pal, J.; Ganguly, M.; Mondal, C.; Roy, A.; Negishi, Y.; Pal, T. Crystal-Plane-Dependent Etching of Cuprous Oxide Nanoparticles of Varied Shapes and Their Application in Visible Light Photocatalysis. *J. Phys. Chem. C* **2013**, *117*, 24640–24653.

(15) Snyder, R. J. and R. L. Introduction to X-ray powder diffractometry. *John Wiley and Sons, New York 1996* **2011**, *11*, 277–278.

(16) Zhang, D. F.; Zhang, H.; Guo, L.; Zheng, K.; Han, X. D.; Zhang, Z. Delicate Control of Crystallographic Facet-Oriented Cu_2O Nanocrystals and the Correlated Adsorption Ability. *J. Mater. Chem* **2009**, *19*, 5220–5225.

(17) Berg, J. M.; Romoser, A.; Banerjee, N.; Zebda, R.; Sayes, C. M. The Relationship between PH and Zeta Potential of ~ 30 Nm Metal Oxide Nanoparticle Suspensions Relevant to in Vitro Toxicological Evaluations. *Nanotoxicology* **2009**, *3*, 276–283.

(18) Tan, J.; Zheng, T.; Yu, Y.; Xu, K. TBHP-Promoted Direct Oxidation Reaction of Benzylic Csp^3-H Bonds to Ketones. *RSC Adv.* **2017**, *7*, 15176–15180.

(19) Wang, H.; Wang, Z.; Huang, H.; Tan, J.; Xu, K. KOtBu-Promoted Oxidation of (Hetero)Benzylic Csp^3-H to Ketones with Molecular Oxygen. *Org. Lett.* **2016**, *18*, 5680–5683.

(20) Yin, M.; Wu, C.-K.; Lou, Y.; Burda, C.; T. Koberstein, J.; Zhu, Y.; O'Brien, S. Copper Oxide Nanocrystals. *J. Am. Chem.l Soc.* **2005**, *127*, 9506–9511.

(21) Robert, T.; Bartel, M.; Offergeld, G. Characterization of Oxygen Species Adsorbed on Copper and Nickel Oxides by X-Ray Photoelectron Spectroscopy. *Surf. Sci.* **1972**, *33*, 123–130.

(22) B. Demissie, T.; H. Hansen, J. Mechanism and Site Selectivity in Visible-Light Photocatalyzed C–H Functionalization: Insights from DFT Calculations. *J. Org. Chem.* **2016**, *81*, 7110–7120.

(23) Chu, C. Y.; Huang, M. H. Facet-Dependent Photocatalytic Properties of Cu_2O Crystals Probed by Using Electron, Hole and Radical Scavengers. *J. Mater. Chem. A* **2017**, *5*, 15116–15123.

(24) T. Sawyer, D.; S. Valentine, J. How Super Is Superoxide? Acc. Chem. Res. **2002**, *14*, 393–400.

(25) H. Huang, M.; Naresh, G.; Chen, H.-S. Facet-Dependent Electrical, Photocatalytic, and Optical Properties of Semiconductor Crystals and Their Implications for Applications. *ACS Appl. Mater. Interfaces* **2017**, *10*, 4–15.

(26) R. Hoffmann, M.; T. Martin, S.; Choi, W.; W. Bahnemann, D. Environmental Applications of Semiconductor Photocatalysis. *Chem. Rev.* **2002**, *95*, 69–96.

(27) Sun, Y.; J. Pignatello, J. Evidence for a Surface Dual Hole-Radical Mechanism in the Titanium Dioxide Photocatalytic Oxidation of 2,4-D. *Environ. Sci. Technol* **2002**, *29*, 2065–2072.

(28) T. Martin, S.; T. Lee, A.; R. Hoffmann, M. Chemical Mechanism of Inorganic Oxidants in the TiO2/UV Process: Increased Rates of Degradation of Chlorinated Hydrocarbons. *Environ. Sci. Technol.* **2002**, *29*, 2567–2573.

(29) Spodine, E.; Manzur, J. Oxygen Insertion in Organic Substrates Catalyzed by Copper Compounds. *Coord. Chem. Rev.* **1992**, *119*, 171–198.

(30) J. Cramer, C.; B. Tolman, W. Mononuclear Cu–O_2 Complexes: Geometries, Spectroscopic Properties, Electronic Structures, and Reactivity. *Acc. Chem. Res.* **2007**, *40*, 601–608.

(31) Trammell, R.; Rajabimoghadam, K.; Garcia-Bosch, I. Copper-Promoted Functionalization of Organic Molecules: From Biologically Relevant Cu/O_2 Model Systems to Organometallic Transformations. *Chem. Rev.* **2019**, *119*, 2954–3031.

(32) Tano, T.; Okubo, Y.; Kunishita, A.; Kubo, M.; Sugimoto, H.; Fujieda, N.; Ogura, T.; Itoh, S. Redox Properties of a Mononuclear Copper(II)-Superoxide Complex. *Inorg. Chem* **2013**, *52*, 10431–10437.

(33) Chen, T.-N.; Kao, J.-C.; Zhong, X.-Y.; Chan, S.-J.; S. Patra, A.; Lo, Y.-C.; H. Huang, M. Facet-Specific Photocatalytic Activity Enhancement of Cu_2O Polyhedra Functionalized with 4-Ethynylanaline Resulting from Band Structure Tuning. *ACS Cent. Sci.* **2020**, *6*, 984–994.

(34) Shah, E.; Vaghasiya, J. V.; Soni, S. S.; Panchal, C. J.; Suryavanshi, P. S.; Chavda, M.; Soni, H. P. Ni Doped ZnS Nanoparticles as Photocatalyst: Can Mixed Phase Be Optimized for Better Performance? *J. Environ. Chem. Eng.* **2016**, *4*, 4708–4718.

(35) Niveditha, C. V.; Fatima, M. J. J.; Sindhu, S. Comprehensive Interfacial Study of Potentio-Dynamically Synthesized Copper Oxide Thin Films for Photoelectrochemical Applications. *J. Electrochem. Soc.* **2016**, *163*,

(36) Li, L.; Zhang, R.; Vinson, J.; L. Shirley, E.; P. Greeley, J.; R. Guest, J.; K. Y. Chan, M. Imaging Catalytic Activation of CO_2 on Cu_2O (110): A First-Principles Study. *Chemistry of Materials* **2018**, *30*, 1912–1923.

(37) Himes, R. A.; Karlin, K. D. Copper–Dioxygen Complex Mediated C–H Bond Oxygenation: Relevance for Particulate Methane Monooxygenase (PMMO). *Curr Opin Chem Biol* **2009**, *13*, 119–131.

(38) Ciano, L.; Davies, G. J.; Tolman, W. B.; Walton, P. H. Bracing Copper for the Catalytic Oxidation of C–H Bonds. *Nat. Catal* **2018**, *1*, 571–577.

(39) Newhouse, T.; Baran, P. S. If C-H Bonds Could Talk: Selective C-H Bond Oxidation. *Angew. Chem. Int. Ed.* **2011**, *50*, 3362–3374.

(40) Luo, Y.-R. *Handbook of Dissociation Energies in Organic Compounds By Yu-Ran Luo (University of South Florida, St. Petersburg). CRC Press LLC: Boca Raton. 2003.*

(41) Zhou, K.; Wang, X.; Sun, X.; Peng, Q.; Li, Y. Enhanced Catalytic Activity of Ceria Nanorods from Well-Defined Reactive Crystal Planes. *J. Catal.* **2005**, *229*, 206–212.