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Lignin into aromatics: Bridging homogeneous and heterogeneous catalysis

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The development of efficient catalytic conversion of lignin into aromatic chemicals remains an important challenge in catalysis due to the amorphous carbon-based inactive property and highly heterogeneous nature of lignin. Potential strategies for the production of aromatics from lignin need to address the issues of lignin solubility as well as of the selective cleavage of the aryl ether bonds. In this lecture, we will discuss our progress in catalytic lignin valorization relating to aforementioned two aspects. In the first part, we will report the selective cleavage of aryl ether in lignin to afford monophenols over tungsten carbide (W_2C) catalysts. The activation mechanisms of different aryl ether bonds over W_2C are deeply explored. On the other hand, synergistic effect between W_2C and a second metal, the effect of the monomer structure on the catalytic performance, and the catalyst stability under liquid phase conditions will be discussed as well. In the second part, selective cleavage of lignin to aromatic compounds catalyzed by methyltrioxorhenium (MTO) without any oxidant (e.g. H_2O_2) and reducing agent (e.g. H_2) is proposed. The introduction of ionic liquids supplies a homogeneous platform which allows the process conducting under mild condition. Microwave irradiation could accelerate the reaction rate and significantly increase the activity. Under optimized conditions, a series of lignin β -O-4 model compounds could afford guaiacol as the primary product with the yields higher than 67%. The possible mechanisms for degradation of lignin is proposed based on IR spectroscopy and NMR results.

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Designing green catalysts using earth-abundant metals: solving the “how-to” and “why” questions using quantum chemistry approaches

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It is a general challenge to design highly active or selective green catalysts using earth-abundant metals. We demonstrated an effective computational approach to deterministically search for optimal binding sites on Cu (100) surface (for catalytic hydrogenation) through the doping of Fe and/or Zn using the inverse molecular design methods. A stable Zn-doped Cu (100) surface was found with optimal binding affinity to H-atoms. We understood the electronic structure cause of the optimal binding sites using orbital-specific binding energy analysis, a new quantum chemistry analysis method here. Overall, we found that the Zn atomic orbitals show less participation in the binding event of H-atoms than the Cu atomic orbitals. In particular, compared to the 3d-orbitals of surface Cu atoms, the 3d-orbitals of surface Zn-atoms show less binding energy contribution and participation, and are much less influenced by the electronic couplings of the media Cu atoms. Our study provides valuable green chemistry insights for the design of green catalysts using earth-abundant metals. Our designed Cu-based earth-abundant alloys may be used for important catalytic hydrogenation applications such as lignin degradation or CO_2 transformation.

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