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Research keywords: (polyoxometalates, theoretical design, DFT study)

The research activity deals with the application of quantum chemistry computational methods to study the properties and chemical reactivity of polyoxometalates (POMs), and solve chemical problems in close collaboration with experimentalists. Currently, the catalytic mechanisms on water oxidation and carbon dioxide reduction reaction by POMs were explored by using density functional theory (DFT) methods. The catalytic activity of POMs and the reaction pathway were analyzed and further catalyst designs are expected based on the relationship between structures and properties.

Possible Collaborations: Josep M. Poblet, Yong Ding, Craig L. Hill

Reference:

[1] Soriano-López, J.; Musaev, D. G.; Hill, C. L.; Galón-Mascarós, J. R.; Carbó, J. J.; Poblet, J. M. *J. Catal.*, 2017, *350*, 56–63.

[2] Liu, R.-J.; Guangjin Zhang, G.-J.; Cao, H.-B.; Zhang, S.-J.; Xie, Y. B.; Haider, A.; Ulrich Kortz, U.; Chen, B.-H.; Naresh S. Dalal, N.-S.; Zhao, Y.-S.; Zhi, L-J.; Wu, C.-X.; Yan, L.-K.; Su, Z.-M.; Keita, B. *Energy Environ. Sci*., 2016, *9*, 1012-1023.