

Electrochemical set-up for HEA synthesis and HER through water-splitting

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## Revolutionizing Chemistry for a Sustainable Future: Pioneering Advances in Organometallic Research by OMCL, IITH



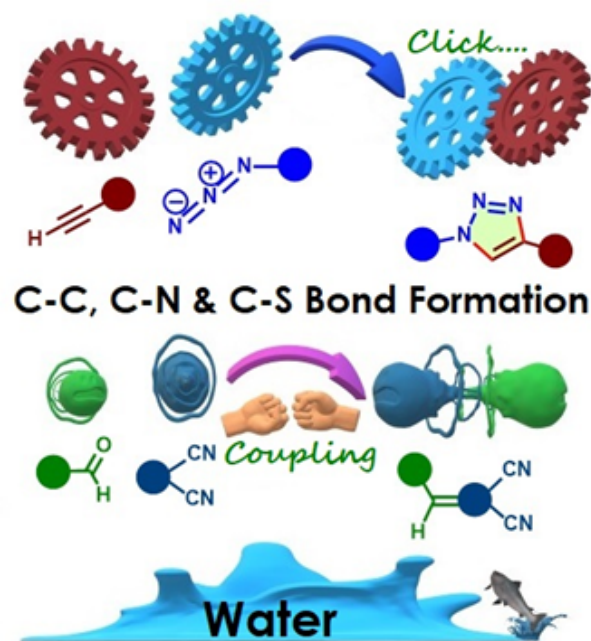
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Our lab is at the forefront of research that unlocks answers to complex questions involving energy, health care, and the environment. We develop significant innovative research and major technological breakthroughs in all aspects of organometallic chemistry and materials, with a particular focus on the important innovation of sustainable methodologies, catalysis, and functional materials.

We contribute to the field of inorganic and organometallic chemistry on fundamental and applied levels by investigating new and efficient ways to activate small molecules and developing catalysts useful in both academic and chemical industries. To accomplish this goal, we systematically develop the hitherto unknown N-heterocyclic carbene (NHC) ligand-supported late transition metal and main group metal catalysts. Novel synthetic methods for metal-NHCs are also being developed within the group, with the aim of making these complexes more attractive for wide-scale use.

We have been Click Chemistry has a great commercial deal in pharmaceutical and life science applications. An azide is added to an alkyne with a copper catalyst. The two reagents click together in a quick and selective manner in the presence of a copper catalyst to result in a single cyclic product. This simple circular economy reaction can be useful in the sustainable synthesis of new drugs through biorthogonal chemistry. This is a key synthetic protocol to generate "clickable" antibodies for cancerous tumours. Based on this technique, antibody-drug conjugates are produced by AstraZeneca and Daiichi Sankyo to replace Herceptin for the treatment of HER2 positive breast cancer.

In this context, we have developed super-fast copper(II) catalyzed click chemistry through a mechanical route to isolate the key pharmaceutical ingredients such as carbazole decorated 1,2,3-triazole derivatives through solvent and additive-free routes. Besides, the regioselective products were isolated within 6 minutes for the first time. This is the only known mild yet fast sustainable approach to isolate the carbazole decorated 1,2,3-triazole derivatives.



GP Group Catalysis Scheme Diagram



Organometallics & Materials Chemistry Lab, Chemistry

(L-R): Mr. Sunham Ojha, Ms. Parkhi Sharma, Dr. Ramesh Karupnaswamy, Dr. Kalaivanan Subramaniam, Mr. Suman Mandal, Prof. G. Prabusankar, Dr. Muneshwar Nandeshwar, Mr. Sabari Veerapathiran, Dr. Mannaem Adinarayana, Dr. Mannarsamy Maruthupandi, and Dr. Vaddamanu Moulali.

Besides, we have developed a straightforward yet scalable approach to isolate another pharmaceutical ingredient, such as ferrocene coumarin. This was achieved through the highly efficient yet sustainable multi-component Knoevenagel condensation approach to isolate the ferrocene coumarin using well-defined, air- and moisture-stable diimine Zn(II) catalysts.

Thioethers are a significant pharma component and one of the challenging molecules to isolate through mild reaction conditions. We have demonstrated the first discrete zinc(II) catalyst-mediated C-S cross-coupling reactions between aryl halides and thiophenols without scrubbing the oxygen and moisture. This methodology is a cheap yet effective alternative for expensive metal catalysts along with a broad substrate scope.

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## Role of catalysts for sustainable future for food, fuels, and commodity products



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The global population is anticipated to double by 2050, with cascading effects on the shrinkage of cultivation land, food and energy resources crisis, and damage increasing environmental pollution. India is already facing a petroleum crisis and relies on ~84% of imports to meet the fuel/chemical demands. Technological innovation must be directed at addressing these futuristic sustainability challenges. The catalysts (bio-, chemo-, and electro-catalysis) will continue to play a pivotal role in the sustainable sourcing of fuels, chemicals, and food/feed products from renewable resources and by valorising/utilizing waste streams and maintaining environment cleanliness. Technological innovations are also progressing radically to produce fuels/chemicals from renewable biomass and organic carbon-rich waste streams in an integrated biorefinery approach. Our current research is directed at producing gasoline, aviation, and diesel range hydrocarbons from renewables or waste carbon sources using chemo-catalysis, thermo-catalytic, or integrated fermentative and chemo-catalytic approaches. Unlike traditional biofuels, these green biofuels are compatible with current infrastructure, have the same fuel mileage, are readily acceptable to customers, and can easily penetrate the market. The aviation sector is expected to grow drastically in the coming years. So, market-ready technology for sustainable aviation fuel (SAF) is thus the need of the hour, as this sector has no alternative energy-sourcing options.

Our recent work demonstrated the proof-of-concept for SAF production from the furanic precursor. The process involves the bioproduction of furanic molecules, followed by its catalytic upgrading into high molecular weight fuel precursors and catalytic deoxygenation to SAF, centred around C14 branched alkanes with better combustion and cold flow properties than n-paraffin and aromatics (Figure-1).

Petroleum and natural gas are the primary raw materials for petrochemicals and fertilizers. Our work is also directed to produce drop-in/platform chemicals/hydrogen from renewable organic resources. Butanediols (BDO) are exemplary platform molecules with tremendous derivative chemistry. The integrated biochemical and chemo-catalytic approach could diversify product opportunities via butanediol, including 1,3-butadiene, methyl ethyl ketone, aromatics, olefins, etc. (Figure-2). Organic carbon wastes and residues from crops, food, industry, and municipality are posing significant environmental problems. Channelling these carbohydrate-rich organic waste carbon streams into value addition products like BDO and its derivatives is a more profitable approach than traditional anaerobic digestion, burning, disposal, or treatment, reducing the effort for waste management and disposal issues.