Tentative Outline

Special Thematic Issue for the journal "Current Catalysis"

Title of the Thematic Issue: Catalytic Degradation of Persistent Organic Pollutants

Section Editor: Dr. Likai Du

- **Scope of the Thematic Issue:**

The catalytic degradation of persistent organic pollutants (POPs) have gained heightened attentions in recent years. The photocatalytic degradation and thermal degradation are comprehensively reviewed. The computational chemistry and machine learning based model were applied to understand the property and catalytic mechanism of POPs.

Keywords:
Reaction mechanism, Organic pollutants, Photocatalysis, P450, microbial enzyme, machine learning

Sub-topics:

- Transition metal model complex and enzymes
- Microplastic aging and degradation
- Photocatalytic Degradation of Organic Pollutants
- Machine-Learning and Quantum Chemistry for POPs.

Tentative titles of the articles:

- Reaction mechanism for photocatalytic degradation of organic pollutants
- Microplastic aging upon the adsorption of sulfonamides and its mechanism
- A stable and easily prepared copper oxide catalyst for degradation of organic pollutants by peroxymonosulfate activation
- Theoretical study of aromatic hydroxylation of the dicopper model complex
- Overview of photocatalytic degradation of organic pollutants
- Modelling interactions between persistent organic pollutants (POPs) and P450s
- Insights into the metabolic mechanism of PBDEs catalyzed by cytochrome P450 enzyme
- Machine-Learning-Based Quantum Chemical Methods in POPs

Schedule:

- Thematic issue submission deadline: 30th-March-23

Contacts:

Sectional Editor Name: Dr. Likai Du
Affiliation: Huazhong Agricultural University, China
Email: likaidu@163.com