Research Interests:

Theoretical and experimental investigation of solid base/acid catalysts for organic reactions

Solid acids and bases play a significant role in the greening of fine and specialty chemicals manufacturing processes. Proton affinity (PAs) and molecular basicities (GBs) of the CaO cluster and CaO modified with protic and aprotic ionic liquids in the gas phase have been calculated at the DFT/B3LYP level with a 6-311++G (d, p) basis set. The investigations of PAs and GBs in the solution phase have been studied by means of SCRF solvent effect computations using PCM solvation model for water solvent.

Proposal of new mechanisms for organic reactions (Experimental & theoretical support)

New mechanism for the Morita–Baylis–Hillman reaction, esterification and biodiesel production was proposed. For the Morita–Baylis–Hillman reaction, we focused on the reaction between acrylonitrile and benzaldehyde, catalyzed by CaO cluster and CaO modified with [Pyr][HSO4] ionic liquid. The mechanism based on the proton transfer was inquired by MP2 and DFT methods with 6-311G++(d, p) basis set combined with IEF-PCM solvent model.

QSPR

Quantitative structure property relationships mathematically link physical or chemical properties with the structure of a molecule. Viscosity, density, surface tension and melting temperature of ionic liquids were modeled using QSPR approach. Linear and nonlinear models were built by means of multiple linear regressions (MLR), multilayer perceptron neural networks (MLP) and using genetic algorithms.

Theoretical and experimental investigation of adsorption of pollutants

Adsorption can be considered to be an effective and low-cost technological process for wastewater treatment. By using Gaussian software and density functional theory at the level of B3LYP/6-31G(d, p), the adsorption of molecules such as phenol, 2-chlorophenol, 4-chlorophenol and 2,4-dichlorophenol over graphene, nitrogen and boron doped graphene sheet are investigated.

Advanced Oxidation Processes (Photocatalysis, Fenton, Electro-Fenton, Photo-electro-Fenton)

Treatment of wastewater which contains toxic and bio-refractory compounds such as dyes, pharmaceuticals, and pesticides has become a serious environmental challenge in the past decade. It sounds that advanced oxidation processes such as photocatalysis, Fenton, electro-Fenton and photo-electro-Fenton have the ability of degradation of these persistent contaminants in the aqueous media based on the formation of hydroxyl radical ($^{\bullet}OH$) as the most powerful oxidant.

Water splitting

Water splitting is a prospective solution for energy and environmental-related problems. Photocatalytic water splitting is an attractive and challenging theme in chemistry. Co2Ni1/g-C_3N_4/rGO can be introduced as a potential powerful photocatalyst for water oxidation reaction under visible light.