Yuhua Zhou

周玉花

Personal Profile

Date of Birth	Mar 6st, 1979.
Place of Birth	Jiangdu, Jiangsu, China
Gender	Female
Marriage Status	Married
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Education

2005.09-present	Ph.D., Quantum Chemistry, Xiamen University.
2002.07-2005.07	M.Sc., Quantum Chemistry, Nankai University.
1998.09-2002.07	B.E., Chemical Engineering and Technology, Xinyang Normal University.

Awards and Honorships

2004-2005	Excellent Graduation Thesis, awarded by Nankai University.
2002-2003	Third Level Scholarship, awarded by Nankai University.
2000-2001	First Level Scholarship, awarded by Xinyang Normal University.
1999-2000	First Level Scholarship, "Excellent student in full aspects", awarded by Xinyang Normal University.
1998-1999	First Level Scholarship, "Excellent student in full aspects", awarded by Xinyang Normal University.

Publications and Researches

2005-present	(1) **Zhou, Y. H.**; Lu, X. * “The Dependence of Intramolecular Charge Transfer within a Donor-σ-Acceptor Dyad on Solvent Polarity: A DFT Study” (in preparing) (2) **Zhou, Y. H.**; Lu, X. * “Intramolecular Electron Transfer Tuned by Hydrogen-Bonding Interactions: A Theoretical Insight” (in preparing) (3) **Zhou, Y. H.**; Lu, X. * “Solvent-controlled Intramolecular Charge Transfer Behavior in Donor-Bridge-Acceptor Dyad Molecules” (in preparing) (4) **Zhou, Y. H.**; Lu, X. * “Weak Electrostatic interactions-induced Intramolecular Charge Transfer Behavior in A-σ-D-σ-A Triad molecule” (in preparing)
2002-2005	(1) **Zhou Y. H.**; Lv P. H.; Wang G. C. * J. Mol.Catal. A-Chem **2006,** *258*, 203-215. (2) Wang G. C.; * **Zhou Y. H.**; Morikawa, Y. et al. J. Phys. Chem. B **2005**, *109*, 12431-12442. (3) Wang G. C.; **Zhou Y. H.**; Nakamura J. J. Chem. Phys. **2005**, *122*, 044707 (4) Wang G. C.; * Jiang L.; **Zhou Y. H.** et al., J. Mol. Struct. **2003,** *634*, 23-30.

Professional skills

English Skills	Have a good command of both spoken and written English. Pass CET 6.
Computer Skills	Linux, Win2K; Gaussian 03 and former versions, Material Studio including $Dmol^3$ and CASTEP, STATE, Chemoffice, Gsview, Molekel, Microsoft Office, Latex *etc*.

Research Experiences and Projects

Investigations on the Process of Methanol Decomposition on Metal Surface based on Plane-wave Method through Energy Band Theory of Solid

A series of decomposition mechanism of methanol molecule on Ni(111) and Ni(100) surfaces have been systematically carried out with DFT calculations based on repeated slab models, the calculations are consistent with available experimental data. The results indicate that methanol molecule is inclined to desorb other than decompose over Ni(111) and Ni(100) surface. However, when at higher temperature, the activation of the O-H bond is the preferable pathway at the first step of dehydrogenation, which is followed by the sequential hydrogen abstracted to form formaldehyde, formyl species, and the final products CO and H. The process of dehydrogenation from methoxy is the rate-limiting step in this pathway. Finally, CO is the most tightly adsorbed species on the surface and may poison the catalyst toward further dehydrogenation.

In addition, the adsorption of related intermediate species, CH_3O, on group IB and some VIII metal surfaces have also been well characterized by the *d*-band center, and the size of the coupling matrix element, which can be treated as the sufficient parameters for understanding the chemadsorption mechanism

The Dependence of Intramolecular Charge Transfer within a series of Donor-σ-Acceptor Dyad Molecules and Acceptor-σ-Donor-σ-Acceptor Triad Molecule on Solvent Polarity, as well as the Short-range Interactions

The study of solvent-induced electron or charge-transfer process represents an extremely active area of chemical research. For the organic donor-σ-acceptor dyad molecules, which often present narrow HOMO-LUMO gap (HLG), it was found that the charge transfer varied depending not only on the electron-withdrawing and donating strength of the substituents in donor and acceptor fragments, respectively, but also on the environment, such as solvent, temperature, light, magnetism et al.

Based on the dielectric continuum solvent model, it was suggested that the dyad molecules with both strong ability of electron-donating and electron-withdrawing, such as TTF-Im-F_4TCNQ, TTF-σ-TCNQ, et al., preferred the charge-separated state in the polar CH_3CN (ε=36.64), DMF (ε=38.25) solvents. The obvious bulk electro-static effect derived from the electronic property of central solute can motivate the charge to transfer from the donor to the acceptor of the solute through the simple continuum solvent models based on SCRF method.

However, the principle does not work in the case of dyad solute molecule with lower electron-withdrawing ability, such as TTF-Q, TTF-6OP. In this condition, the short-range solvent-solute interactions are playing more essential role than the bulk solvent effect, such as the specific hydrogen-bonding between protic solvent and solute molecules. In order to describe such kind of interactions, the discrete-cluster models are useful for investigations of the ICT behaviors, along with the state interconversion resulted from the short-range interactions, which provides us more insight into the solvent perturbation on the chemical properties of solute.

Considering the "S" type triad molecule, TCNQ-σ-TTF-σ-TCNQ, the very small polarity induced little perturbations of the "solvent field", which has little effect on the properties of central solute molecules, although it has both strong electron-donating and electron-withdrawing fragments as in dyad TTF-σ-TCNQ molecule. The strong dependence of the electronic state on the polarity of the surrounding was well described by using the discrete-cluster models, which indicated the short-range dipole-dipole interaction between the polar solvent and the triad molecule played the dominant role in inducing the ICT characters.

On all accounts, suitable solvent model would provide more insight into the mechanism of unprecedented solvatochromism of the solvent-induced ICT behavior in a serious of dyad and triad molecules.

Referees

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