

# Chinese Journal of Chemical Physics

VOLUME 27, NUMBER 1, FEBRUARY 27, 2014

## ARTICLES

- 1 **CO<sub>2</sub> Pressure Shift and Broadening of Water Lines Near 790 nm**  
Yan Lu, Xin-fei Li, An-wen Liu\*, Shui-ming Hu
- 5 **Infrared Spectroscopy of CO Isolated in Solid Nitrogen Matrix**  
Lei Wu, Ricardo Lambo\*, Yan Tan, An-wen Liu, Shui-ming Hu
- 9 **Theoretical Investigations on Graphite Oxide Immersed in Water or Methanol**  
Wan-wan Geng, Wen-hui Zhao, Lan-feng Yuan\*
- 15 **New Hexagonal-rhombic Trilayer Ice Structure Confined between Hydrophobic Plates**  
Min Jia, Wen-hui Zhao, Lan-feng Yuan\*
- 20 **O<sub>2</sub>, CO<sub>2</sub>, and H<sub>2</sub>O Chemisorption on UN(001) Surface: Density Functional Theory Study**  
Ru-song Li\*, Bin He, Fei Wang, Peng Xu, Hua Wang
- 29 **GPCR A<sub>2A</sub>AR Agonist Binding and Induced Conformation Changes of Functional Switches**  
Xue-qin Pang, Jian-yong Liu\*
- 39 **Theoretical Study of Reagent Rotational Excitation Effect on the Stereodynamics of H+LiF→HF+Li Reaction**  
Ting-xian Xie, Ying-ying Zhang, Ying Shi\*, Ming-xing Jin
- 45 **Quantum Chemical Studies on Structure and Detonation Performance of Bis(2,2-dinitropropyl ethylene)formal**  
Shu-qin Yan, Xiao-hong Li\*
- 51 **Experimental and Theoretical Investigation on Excited State Intramolecular Proton Transfer Coupled Charge Transfer Reaction of Baicalein**  
Shan-shan Hu, Kun Liu, Qian-qian Ding, Wei Peng\*, Mao-du Chen\*
- 57 **Anisotropy of Thermal-expansion for β-Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine: Quantum Chemistry Calculation and Molecular Dynamics Simulation**  
Wen Qian, Chao-yang Zhang, Yuan-jie Shu\*, Ying Xiong, He-hou Zong, Wei-bin Zhang
- 63 **Kinetic Implication from Temperature Effect on Hydrogen Evolution Reaction at Ag Electrode**  
Jing Kang, Chu-hong Lin, Yao Yao, Yan-xia Chen\*
- 69 **High Pressure Structural Instability and Thermal Properties of Rutile TiO<sub>2</sub> from First-principles**  
Cui-e Hu, Zhao-yi Zeng\*, Chun-yang Kong, Yu-ting Cui, Lin Zhang, Ling-cang Cai
- 75 **Effects of Rotational Isomerism and Bond Length Alternation on Optical Spectra of FTC Chromophore in Solution**  
Ke Zhao\*, Guang-chao Han, Li-li Zhang, Hai-hong Jia
- 82 **Effect of Ar<sup>+</sup>, He<sup>+</sup>, and S<sup>+</sup> Irradiation on n-InP Single Crystal**  
Jing-yu Hu, Waqas Mahmood, Qing Zhao\*
- 87 **Spontaneous Cracking of Graphite Oxide Sheet on Oxygen Deficient ZnO Film**  
Jin-yang Liu, Hong-bin Cai, Huan-yi Ding, Kun Zhang, Nan Pan, Xiao-ping Wang\*
- 92 **Conversion of Pretreated Biomass into Levulinic Acid via Continuous Extraction at Atmosphere Pressure**  
Ming-hui Fan, Li-feng Yan\*

(Contents continued on inside back cover)

(Contents continued from outside back cover)

- 99 Hierarchical Radial Co<sub>3</sub>O<sub>4</sub> Microcrystal and Application in Gas Sensor**  
Xin-xin Yu, Xian-song Liu, Ming-zai Wu\*, Zhao-qi Sun, Guang Li, Xiao-shuang Chen
- 103 Theoretical Study on the High-Temperature  $P\bar{6}$  and  $P\bar{6}'$  Phases of Si<sub>3</sub>N<sub>4</sub>: A Tool to Aid in Ceramics Development**  
Ben-hai Yu, Dong Chen\*
- 109 Investigation on Excited-State Photophysical Characteristics of Low Bandgap Polymer APFO3**  
Li-li Qu, Ying-hui Wang\*, Zhi-hui Kang, Yu-guang Ma, Han-zhuang Zhang\*
- 115 Interaction Study between DNA and Histone Proteins on Single-molecule Level using Atomic Force Microscopy**  
Yu-ying Liu\*, Peng-ye Wang, Shuo-xing Dou, Hong-feng Lv
- 121 Alumina Photonic Crystals with Defect Modes for Sensor Application**  
Peng Yan, Guang-Tao Fei\*, Hui Li, Guo-liang Shang, Bing Wu, Li-de Zhang
- i Chinese Abstracts**