

Chinese Journal of Chemical Physics

VOLUME 27, NUMBER 4, AUGUST 27, 2014

ARTICLES

- 373 **Global Potential Energy Surface for the $\text{H}+\text{CH}_4\leftrightarrow\text{H}_2+\text{CH}_3$ Reaction using Neural Networks**
Xin Xu, Jun Chen, Dong H. Zhang*
- 380 **Molecular Dynamics Study on Configuration Energy and Radial Distribution Functions of Ammonium Dihydrogen Phosphates Solution**
Kun Wang*, Ya-fan Zhao, Gui-wu Lu, Yu-liang Wang, Ju-na Chen, De-zhi Su
- 387 **Elasticity and Thermodynamic Properties of EuS Related to Phase Transition**
Qiang Liu, Feng Peng*
- 394 **Uniform B-C-N Ternary Monolayer from Non-Metal Filled $g\text{-C}_3\text{N}_4$ Sheet**
Na Zhang, Xiao-jun Wu*
- 399 **Insights into Elastic and Thermodynamics Properties of Binary Intermetallics in Ni-Al Alloys under Extreme Condition: Full-Electronic Quasi-Harmonic Study**
Yong-song Luo, Yu-ping Cang, Dong Chen*
- 407 **Negative Differential Resistance of Au-MgB₂-Au Nanoscale Junctions**
Fu-ti Liu, Yan Cheng*, Xiang-rong Chen
- 412 **Molecular Dynamic Simulation of Melting Points of *trans*-1,4,5,8- tetranitro-1,4,5,8-tetraazadacalin (TNAD) with Some Propellants**
Xiao-hong Li*, Xue-hai Ju*
- 419 **Self-assembly of Binary Particles with Electrostatic and van der Waals Interactions**
Yan Li, Hua-ping Li, Xue-hao He*
- 428 **Hydrothermal Synthesis and Efficient Visible Light Photocatalytic Properties of InVO₄ Hierarchical Microspheres and InVO₄ Nanowires**
Xue Lin*, Shi-duo Zhao, Xiao-yu Guo, Xin Gao, Jiu-jing Shi, Yi-li Liu, Hong-ju Zhai, Qing-wei Wang*
- 433 **Promotion of Ni/MCM-41 Catalyst for Hydrogenation of Naphthalene by co-Impregnation with Polyols**
Song-bai Qiu, Yu-jing Weng, Yu-ping Li, Long-long Ma, Qi Zhang, Tie-jun Wang*
- 439 **Preparation of TiO₂/Bi₂O₃ Microfibers and Their Photocatalytic Activity**
Zhan-ying Ma*, Ling-juan Deng, Xiao-bo Li, Guang Fan*
- 445 **Effect of Molybdenum Doping on Oxygen Permeation Properties and Chemical Stability of SrCo_{0.8}Fe_{0.2}O_{3- δ}**
Chun-lin Song*, Shu-min Fang*
- 450 **Effect of Surfactant-Induced Modifications on CuCoMn Catalysts for Higher Alcohol Synthesis**
Zhao-xia Zhang, Pei-yan Bi, Pei-wen Jiang, Quan-xin Li*
- 457 **Composite Cathode based on Mn-doped Perovskite Niobate-Titanate for Efficient Steam Electrolysis**
Jun Zhang, Kui Xie*, Yuan-xin Li, Wen-tao Qi, Cong Ruan, Yu-cheng Wu*
- 465 **Nanocomposites of Polydiacetylene and Rare Earth Ions with Reversible Thermochromism**
Kai-yu Fu, Dao-yong Chen*
- 471 **Phase Transition Behaviour of VO₂ Nanorods**
Ying Luo, Ming Li, Guang-hai Li*

(Contents continued on inside back cover)

(Contents continued from outside back cover)

- 475 **Exchange Bias Effect in Phase Separated $\text{La}_{0.33}\text{Pr}_{0.34}\text{Ca}_{0.33}\text{MnO}_3$ Thin Films**
Hui Li, Lin Li, Long Cheng, Hai-xing Liang, Chang-gan Zeng*
- 479 **Kinetics Study on O_2 Adsorption and OH_{ad} Desorption at Pt(111), Its Implication to Oxygen Reduction Reaction Kinetics**
Fan Yang, Ling-wen Liao, Ming-fang Li, Dong Mei, Yan-xia Chen*
- 485 **Gelled Ionic Liquid/PMMA Polymer Electrolyte Prepared by Radical Polymerization**
Li-bo Li*, Shuo Yang, Jie-si Li, Shao-wen Guo
- 491 **Corrosion Study on Tantalum in Anhydrous Ethanol**
Hai-ping Yang*, Mo-tang Tang, Bi-hui Li
- ii **Chinese Abstracts**