Special Topic of “the Young Scientist Forum on Chemical Physics: Theoretical and Computational Chemistry Workshop 2020”
Guest Editor: Qiang Shi

497 Generalized Quantum Master Equation: A Tutorial Review and Recent Advances
Dominikus Brian, Xiang Sun

525 Structured Eigenvalue Problems in Electronic Structure Methods from a Unified Perspective
Zhendong Li

532 Super-exchange and Exchange-Enhanced Reactivity in Fe₄S₄ Mediated Activation of SAM
by Radical SAM Enzymes
Jian-qiang Feng, Bin-ju Wang

541 Constrained Density Functional Theory Plus the Hubbard U Correction Approach for
the Electronic Polaron Mobility: A Case Study of TiO₂
Yue-Chao Wang, Hong Jiang

552 KSSOLV-GPU: an Efficient GPU-enabled MATLAB Toolbox for Solving the Kohn-Sham
Equations within Density Functional Theory in Plane-Wave Basis Set
Zhen-lin Zhang, Shi-zhe Jiao, Jie-lan Li, Wen-tiao Wu, Ling-yun Wan, Xin-ming Qin, Wei Hu
Jin-long Yang

565 Time-Dependent Density Matrix Renormalization Group Coupled with n-Mode
Representation Potentials for the Excited State Radiationless Decay Rate: Formalism
and Application to Azulene
Jia-jun Ren, Yuan-heng Wang, Wei-tang Li, Tong Jiang, Zhi-gang Shuai

583 Recent Implementations in LASP 3.0: Global Neural Network Potential with Multiple
Elements and Better Long-Range Description
Pei-lin Kang, Cheng Shang, Zhi-pan Liu
Special Topic of “the Young Scientist Forum on Chemical Physics: Ultrafast Dynamics of Photoelectric Conversion Workshop 2020”
Guest Editor: Shengye Jin

591 Dynamic Variation of Excitonic Coupling in Excited Bilayer Graphene Quantum Dots
Yu Wang, Xin-jing Zhao, Rong-Jing Wei, Gui-jie Liang, Kang Wang, Yuan-zhi Tan*, Ye Yang*

598 Coherent Vibrational Dynamics of \([Au_{25}(SR)_{18}]^-\) Nanoclusters
Jie Kong, Yan-zhen Wu, Meng Zhou*

605 Direct Observation of Electron-Vibration Coupling at MXene-Solvent Interface
Yan-jun Xu, He-yuan Liu, Hai-long Chen*

613 Accelerated Interfacial Charge Transfer in Br-Gradient MAPbI\(_{3-x}Br_x\) Perovskite Thin Films
Ye-jun Xiao, Jun-xue Liu, Jing Leng*, Bo-ning Wu, Shengye Jin*

621 Long Chain Fatty Acid Affects Excited State Branching in Bilirubin-Human Serum Protein Complex
Yang-yi Liu, Hai-feng Pan*, Jian-hua Xu, Jin-quan Chen*

******************************************************************************

ARTICLE

628 Surface, Size and Thermal Effects in Alkali Metal with Core-Electron Binding-energy Shifts
Wen-huan Zhu, Zhong-kai Huang*, Mao-lin Bo*, Jin Huang, Cheng Peng, Hai Liu*

639 Reduction of Dimerization Tendency Due to the Decrease in Hybridization Index by
Inclusion of 4s and 4p Semicore States as Valence States in Mo\(_n\) (\(n=2–18\)) Clusters:
A First-Principles Study
Zhao-ye Gong, Zhi-qiang Sun, Yan-wen Ding, Shuai Zhang, Zhen-long Lv, Xiao-fei Wang, Li-ben Li,
Hai-sheng Li*

Chinese Abstracts