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丁迅雷, 男, 1980年9月生, 汉族。长期从事理论物理化学研究工作, 在团簇、表面、材料体系的结构、性质、反应机理等研究方面取得了一系列原创性成果。共发表SCI论文80余篇, 其中第一作者或通讯作者SCI论文36篇, 单篇论文最高他引超过100次。先后主持三项国家自然科学基金(重大研究计划培育项目、面上项目、青年项目)、中央高校基本科研业务费基金重点项目、教育部留学回国人员基金、中国博士后基金、中科院科研基金等多个科研项目, 并获得学校“青年骨干教师支持计划”和“优青培育计划”的支持。

教育经历

1999/08-2004/11 中国科学技术大学, 化学物理系, 博士, 导师: 杨金龙

1995/09-1999/07 中国科学技术大学, 少年班, 物理学, 学士

工作经历

2018/07-至今 可再生能源学院, 博士生导师

2013/06-至今 华北电力大学, 数理学院, 教授

2007/11-2013/06 中科院化学所, 动态与稳态结构国家重点实验室, 副研究员

2005/11-2007/11 意大利国家模拟中心CNR-INFM DEMOCRITOS, 博士后

2005/7-2005/9 国家自然科学基金委员会国际合作交流项目资助, 意大利国际理论物理中心(ICTP), 交流学习

2004/11-2005/10 合肥微尺度物质科学国家实验室, 博士后

目前主要研究方向:

- (1) 单原子催化体系的理论模拟。
- (2) 太阳能电池相关材料的理论模拟。
- (3) 团簇结构及其物理化学性质。

近期代表性论文:

- 1、Ding, X.-L.; Liao, H.-L.; Zhang, Y.; Chen, Y.-M.; Wang, D.; Wang, Y.-Y.; Zhang, H.-Y., Geometric and Electronic Properties of Gold Clusters Doped with a Single Oxygen Atom, *Phys. Chem. Chem. Phys.*, 18 (41), 28960-28972, 2016.
- 2、Ding, X.-L.; Wang, D.; Li, R.-J.; Liao, H.-L.; Zhang, Y.; Zhang, H.-Y., Adsorption of a Single Gold or Silver Atom on Vanadium Oxide Clusters, *Phys. Chem. Chem. Phys.*, 18 (14), 9497-9503, 2016.
- 3、Ding, X.-L.; Wang, D.; Wu, X.-N.; Li, Z.-Y.; Zhao, Y.-X.; He, S.-G., High Reactivity of Nanosized Niobium Oxide Cluster Cations in Methane Activation: A Comparison with Vanadium Oxides, *J. Chem. Phys.*, 143 (12), 124312, 2015.
- 4、Ding, X.-L.; Li, Z.-Y.; Meng, J.-H.; Zhao, Y.-X.; He, S.-G., Density-Functional Global Optimization of $(\text{La}_2\text{O}_3)_N$ Clusters, *J. Chem. Phys.*, 137 (21), 214311, 2012.
- 5、Ding, X.-L.; Wu, X.-N.; Zhao, Y.-X.; He, S.-G., C-H Bond Activation by Oxygen-Centered Radicals over Atomic Clusters, *Acc. Chem. Res.*, 45 (3), 382-390, 2012.
- 6、Gao, Z.; Sun, Y.; Li, M.; Yang, W.; Ding, X., Adsorption Sensitivity of Fe Decorated Different Graphene Supports toward Toxic Gas Molecules (CO and NO), *Appl. Surf. Sci.*, 456, 351-359, 2018.
- 7、Gao, Z.-Y.; Yang, W.-J.; Ding, X.-L.; Lv, G.; Yan, W.-P., Support Effects on Adsorption and Catalytic Activation of O_2 in Single Atom Iron Catalysts with Graphene-Based Substrates, *Phys. Chem. Chem. Phys.*, 20 (10), 7333-7341, 2018.
- 8、Wang, Y.-Y.; Deng, J.-J.; Wang, X.; Che, J.-T.; Ding, X.-L., Small Stoichiometric $(\text{MoS}_2)_N$ Clusters with the 1T Phase, *Phys. Chem. Chem. Phys.*, 20 (9), 6365-6373, 2018.

- 9、Zhang, Y.; Li, Z.-Y.; Zhao, Y.-X.; Li, H.-F.; Ding, X.-L.; Zhang, H.-Y.; He, S.-G., H₂ Oxidation Mediated by Au₁-Doped Vanadium Oxide Cluster Cation AuV₂O₅⁺: A Comparative Study with AuCe₂O₄⁺, *J. Phys. Chem. A*, 121 (21), 4069-4075, 2017.
- 10、Ling, J.-F.; Ding, X.-L.; Li, Z.-Y.; Yang, J.-L., First-Principles Study of Molecular Clusters Formed by Nitric Acid and Ammonia, *J. Phys. Chem. A*, 121 (3), 661-668, 2017.
- 11、Zhang, H.-X.; Ding, X.-L., DFT Investigations on AuVO₃⁺, a Barrier-Free Catalyst for Oxidation of CO with O₂, *Chem. Phys.*, 475, 69-76, 2016.
- 12、Chen, Y.-J.; Yue, L.; Li, Z.-H.; Ding, X.-L.; Wang, L.; Dai, X.-H.; Fang, X.; Pan, Y.-J.; Ding, C.-F., Investigation of Protonated and Sodiated Leucine-Enkephalin by Hydrogen-Deuterium Exchange and Theoretical Calculations, *Anal. Methods*, 7 (13), 5551-5556, 2015.
- 13、Wu, X.-N.; Ding, X.-L.; Li, Z.-Y.; Zhao, Y.-X.; He, S.-G., Hydrogen Atom Abstraction from CH₄ by Nanosized Vanadium Oxide Cluster Cations, *J. Phys. Chem. C*, 118 (41), 24062-24071, 2014.
- 14、Zheng, B.; Hou, B.; Wang, Z.-X.; Yi, P.-G.; Wu, J.-Y.; Ding, X.-L., Theoretical Characters and Nature of the Intermolecular Lithium Bonded Interactions B...LiCN/LiNC (B = Pyridine, Furan and Thiophene), *Comput. Theor. Chem.*, 1017, 153-158, 2013.
- 15、Ma, J.-B.; Zhao, Y.-X.; He, S.-G.; Ding, X.-L., Experimental and Theoretical Study of the Reactions between Vanadium Oxide Cluster Cations and Water, *J. Phys. Chem. A*, 116 (9), 2049-2054, 2012.

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