

Dong Tian

■ E-mail: dong.tian@aliyun.com/dt2647@columbia.edu

■ Address: State Key Laboratory of Complex Nonferrous Metal Resources Clean Utilization, Kunming University of Science and Technology. No. 253, Xuefu Road, Wuhua District, 650093, Kunming, Yunnan, P. R. China

■ Google Scholar: <https://scholar.google.com.hk/citations?user=vIyfsn0AAAAJ&hl=zh-CN>

Research Interests:

Study the reaction mechanism of thermochemical (alkane conversion and CO₂ hydrogenation) and electrochemical (hydrogen evolution reaction and CO₂ reduction reaction) on metals and supported metal (e.g. oxide supported metals, carbide and nitride supported metals) catalysts by DFT calculations.

Publications:

1. **Dong Tian**, Chunhua Zeng, Yunchang Fu, Hua Wang, Hongchun Luo, Chao Xiang, Yonggang Wei, Kongzhai Li, Xing Zhu. A DFT study of the structural, electronic and optical properties of transition metal doped fluorite oxides: Ce_{0.75}M_{0.25}O₂ (M= Fe, Co, Ni), Solid State Communications, 231-232 (2016) 68–79.
2. **Dong Tian**, Chunhua Zeng, Hua Wang, Hongchun Luo, Xianming Cheng, Chao Xiang, Yonggang Wei, Kongzhai Li, Xing Zhu. Performance of cubic ZrO₂ doped CeO₂: First-principles investigation on elastic, electronic and optical properties of Ce_{1-x}Zr_xO₂, Journal of Alloys and Compounds, 671 (2016) 208-219.
3. **Dong Tian**, Chunhua Zeng, Hua Wang, Xianming Cheng, Yane Zheng, Chao Xiang, Yonggang Wei, Kongzhai Li, Xing Zhu. Effect of transition metal Fe adsorption on CeO₂ (110) surface in the methane activation and oxygen vacancy formation: A density functional theory study, Applied Surface Science, 416 (2017) 547–564.
4. **Dong Tian**, Kongzhai Li, Yonggang Wei, Xing Zhu, Chunhua Zeng, Xianming

- Cheng, Yane Zheng, Hua Wang. DFT insight into the oxygen vacancies formation and CH₄ activation over CeO₂ surfaces modified by transition metals (Fe, Co and Ni), *Physical Chemistry Chemical Physics*, 20 (17), 11912-11929, 2018.
5. Yufei Xue, **Dong Tian**, Dexin Zhang, Chunhua Zeng, Yunchang Fu, Kongzhai Li, Hua Wang, Yafang Tian. The mechanism of photocatalyst and the effects of co-doping CeO₂ on refractive index and reflectivity from DFT calculation, *Computational Materials Science* 158, 197-208, 2019.
 6. Xianming Cheng, Kongzhai Li, Hua Wang, Xing Zhu, Yonggang Wei, Zhouhang Li, MinZheng, **Dong Tian**. Chemical looping combustion of methane in a large laboratory unit: Model study on the reactivity and effective utilization of typical oxygen carriers, *Chemical Engineering Journal*, 2017, 328: 382-396.
 7. Xianming Cheng, Kongzhai Li, Yonggang Wei, Xing Zhu, **Dong Tian**. Modification of KNO₃ on the reducibility and reactivity of Fe₂O₃-based oxygen carriers for chemical-looping combustion of methane. *The Canadian Journal of Chemical Engineering*, 2017, 95: 1569–1578.
 8. Xing Zhu, Congzhi Shi, Kongzhai Li, Kang Zhai, Hua Wang, Yonggang Wei, **Dong Tian**, Chunhua Zeng. Water splitting for hydrogen generation over lanthanum-calcium-iron perovskite-type membrane driven by reducing atmosphere, *International Journal of Hydrogen Energy*, 2017, 42: 19776-19787.
 9. Yane Zheng, Kongzhai Li, Hua Wang, Yuhao Wang, **Dong Tian**, Xing Zhu, Yonggang Wei, Chunhua Zeng, Yongming Luo. Structure dependence and reaction mechanism of CO oxidation: A model study on microporous CeO₂ and CeO₂-ZrO₂ catalysts, *Journal of Catalysis*, 2016, 344: 365–377.
 10. Yane Zheng, Kongzhai Li, Hua Wang, **Dong Tian**, Yuhao Wang, Xing Zhu, Yonggang Wei, Min Zheng, Yongming Luo. Designed oxygen carriers from macroporous LaFeO₃ supported CeO₂ for chemical-looping reforming of

- methane, Applied Catalysis B: Environmental, 2017, 202: 51–63.
11. Danyang Li, Kongzhai Li, Ruidong Xu, Hua Wang, **Dong Tian**, Yonggang Wei, Xing Zhu, Chunhun Zeng, Liangpeng Zeng. Ce_{1-x}Fe_xO_{2-δ} catalysts for catalytic methane combustion: Role of oxygen vacancy and structural dependence, Catalysis Today, 318, 73-85
 12. Hongchun Luo, **Dong Tian**, Chunhua Zeng, Yunchang Fu, Hua Wang. First-principles study the behavior of oxygen vacancy on the surface of ZrO₂ and Zr_{0.97}M_{0.03}O₂, Computational Condensed Matter 11 (2017) 1-10.
 13. Chao Xiang, Jianxiong Zhang, Yun Lu, **Dong Tian**, Cheng Peng, Electronic and optical properties of the spine oxides Mg_xZn_{1-x}Al₂O₄ by first-principles calculations, Materiali in tehnologije, 51 (5), 735-743.
 14. Xianming Cheng, Kongzhai Li, Xing Zhu, Yonggang Wei, Zhouhang Li, Yanhui Long, Min Zheng, **Dong Tian**, Hua Wang, Enhanced performance of chemical looping combustion of methane by combining oxygen carriers via optimizing the stacking sequences, Applied energy, 230, 696-711.
 15. Danyang Li, Kongzhai Li, Ruidong Xu, Xing Zhu, Yonggang Wei, **Dong Tian**, Xianming Cheng, Hua Wang, Enhanced CH₄ and CO Oxidation over Ce_{1-x}Fe_xO_{2-δ} Hybrid Catalysts by Tuning the Lattice Distortion and the State of Surface Iron Species, ACS applied materials & interfaces 11 (21), 19227-19241, 2019.

Awards:

1. “National scholarship for Doctoral candidate of the People's Republic of China”, 2017.11.
2. “Provincial government scholarship for Doctoral candidate in Yunnan province”, 2016.12.
3. “Academic newcomer award of Doctoral candidate in Yunnan province”, 2016.10.
4. “National metallurgy university (material, metallurgy, machinery) postgraduate

- BBS second prize”, 2017.07.
5. “First class scholarship of Kunming University of Science and Technology”, 2016
 6. “First class scholarship of Kunming University of Science and Technology”, 2017.
 7. “Research and international exchange program high level paper award of Kunming University of Science and Technology”, 2017.10.
 8. “Outstanding graduate student party member of Kunming University of Science and Technology”, 2017. 06.
 9. “Outstanding student leaders in Weinan Normal University”, 2013.06.
 10. “Students innovation and entrepreneurship President award of Weinan Normal University”, 2013.05.
 11. “Merit student of Weinan Normal University”, 2012.12.
 12. “Principal scholarship of Weinan Normal University”, 2011.09