

主要科技成果目录（288 篇研究论文）

- 1) Kang Li, Jing Li, Pu Wang*, and **Yong Pei***. Theoretical Insights on the Regulatory Mechanisms of Structure and Doping on the Photoluminescence of Ligand Protected Gold Nanoclusters[J]. *Accounts of Chemical Research*, 2026, **59**(5): 713-725.
- 2) Jun Pang, Xinyu Bai, Junjie Dai, Sijie Liu, Shuangfeng Yin*, **Yong Pei***, Rong Tan* Atmospheric CO₂-to-acetaldehyde artificial photosynthesis in metallo hydrogen-bonded organic frameworks *Nat. Commun.* 2026, 17: 8583.
- 3) W. Li,* P. Zhang, Z. Yang, S. Gumber, **Y. Pei***, O. V. Prezhdo* Ultrafast Auger-Mediated Interlayer Electron Transfer in 2D Perovskites: Ab Initio Quantum Dynamics Simulation *Nano Letters* 2026, 26: 10587-10595
- 4) Mengdan Luo, Hongyan Zeng, Yang Zhang*, Mingjun Jing, Tianjing Wu*, Honghui Hu, **Yong Pei***, Lijie Liu, Yujie Huang, Hongshuai Hou*, Xianyou Wang, and Xiaobo Ji. Reaction mechanisms and practical applications of Si-X compounds (X=O, C, OC, P, N) toward next-generation LIB anodes: The role of host and modifier[J]. *Coordination Chemistry Reviews*, 2026, **565**: 218117.
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- 8) Honghui Hu, Yu Mei, Mingjun Jing, Jinyang Wu*, Tianjing Wu, Jinzhi Yuan, Zichun Zhang, **Yong Pei***, Cheng Cheng, Yujie Huang, Hongshuai Hou*, Xianyou Wang, and Xiaobo Ji*. Programmable Diacetylene-Bridged Cyclotetrathiophenes With Nonplanar π -Expanded Skeleton for Electrochemical Sodium Storage[J]. *Angewandte Chemie International Edition*, 2026, **65**(21): e4610174.
- 9) Lirong Xia, Kehao Zhang, and **Yong Pei***. Unraveling defect-mediated ion transport behavior in anti-perovskite solid-state electrolytes via machine learning molecular dynamics simulations[J]. *Physical Chemistry Chemical Physics*, 2026, **28**(17): 10698-10707.

- 10) Kang Li, Pu Wang*, and **Yong Pei***. Photoluminescence of ligand-protected gold nanoclusters: progress in experimental and theoretical studies[J]. *Chemical Science*, 2026, **17**(14): 6907-6923.
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