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Education

2019. 03 - Current: **Postdoctoral researcher**, in Material Chemistry, Institute of Functional Nano & Soft Materials (FUNSOM), Soochow University

Supervisor: Prof. Dr. Tao Cheng

2017. 02 - 2019.02: **Visiting researcher**, Materials and Process Simulation Center, California Institute of Technology

Supervisor: Prof. Dr. William A. Goddard III

2014. 03 -2018. 12:**Doctor of Philosophy**, in Applied Chemistry, College of Chemistry and Molecular Engineering, Nanjing Tech University

Supervisor: Prof. Dr. Xiao-Ming Ren

Thesis title: *Experimental and theoretical investigations of cation conformation dependence of crystal structures, magnetic and electric properties in transition metal dithiolene ionic crystals*

2011. 09 - 2014. 03:**Master of Science**, in Organic Chemistry, College of Science, Nanjing Tech University

Supervisor: Prof. Dr. Xiao-Ming Ren

2007. 09 - 2011. 06:**Bachelor of Science**, in Material Chemistry, School of Chemistry and Chemical Engineering, Anqing Normal University

Thesis title: *Synthesis, characterization and magnetic properties of*

[Ni(dmit)$_2$]-based molecular spin-ladder materials

Publications

Manuscripts prepared

1. Pengtang Wang,[#] **Hao Yang**,[#] Yong Xu,[#] *et. al.,* A synergized Cu/Pb core/shell electrocatalyst for high-efficiency CO_2 reduction to C_2+ liquids, *ACS Nano*, 2020, revised.
2. **Hao Yang**, Tao Cheng, William A. Goddard III, London dispersion corrections to density functional theory for transition-metals based on fitting to experimental temperature-programmed desorption of benzene monolayers, *J. Phys. Chem. Lett.*, 2020, revised.
3. Kailei Cao,[#] **Hao Yang**,[#] Shuxing Bai, *et. al.,* Efficient direct H_2O_2 synthesis enabled by PdPb nanorings via inhibiting the O-O bond cleavage in O_2 and H_2O_2, *ACS Catal.*, 2020, submitted.
4. Jianghao Wang,[#] **Hao Yang**,[#] Qianqian Liu, *et. al.,* Fastening Br^- ions at copper-molecule interface enables highly efficient electroreduction of CO_2 to ethanol, *ACS Energy Lett.,* 2020, submitted.
5. Miao Wang,[#] **Hao Yang**,[#] Jinan Shi, *et. al.,* Alloying nickel with molybdenum significantly accelerates bifunctional hydrogen electrocatalysis in alkaline solution, *Angew. Chem.*, 2020, submitted.
6. **Hao Yang**,[#] Fabio R. Negreiros,[#] Qintao Sun, *et. al.,* XPS prediction for reaction intermediates in CO_2RR/CORR on Cu(100) during operando electrocatalysis process. 2020, prepared.

Journal Articles **(updated: 2020-11-14)**

31. Yonggang Feng,[#] **Hao Yang**,[#] Ying Zhang, *et. al.,* Te-doped Pd nanocrystal for electrochemical urea production by efficiently coupling carbon dioxide reduction with nitrite reduction, *Nano Lett.,* 2020, **20**, 8282-8289.([#]Co-First Author.)
30. Yifan Ye,[#] Jin Qian,[#] **Hao Yang**,[#] *et. al.,* Synergy between a ailver-copper surface alloy composition and carbon dioxide adsorption and activation, *ACS Appl. Mater.*

Interfaces, 2020, **12**, 25374-25382. ([#]Co-First Author.)

29. Chaochao Zhang,[#] **Hao Yang**,[#] Dan Zhong,[#] *et. al*., A yolk–shell structured metal-organic framework with encapsulated iron-porphyrin and its derived bimetallic nitrogen-doped porous carbon for an efficient oxygen reduction reaction, *J. Mater. Chem. A*, 2020, **8**, 9536-9544. (Highlighted as inside front cover, [#]Co-First Author.)
28. Qikui Fan,[#] **Hao Yang**,[#] Juan Ge, *et. al*., Customizable ligand exchange for tailored surface property of noble metal nanocrystals, *Research*, 2020, https://doi.org/10.34133/2020/2131806. ([#]Co-First Author.)
27. Fenglou Ni, **Hao Yang**, Yunzhou Wen, *et. al*., N-modulated Cu^{+} for efficient electrochemical carbon monoxide reduction to acetate, Sci. China Mater., 2020, https://doi.org/10.1007/s40843-020-1440-6.
26. Haipeng Bai, Tao Cheng, Shangyu Li, Zhenyu Zhou, Hao Yang, *et. al.*, Controllable CO adsorption determines ethylene and methane productions from CO_2 electroreduction, *Sci. Bull.*, 2020, https://doi.org/10.1016/j.scib.2020.06.023.
25. Xuchun Wang, Miao Xie, Fenglei Lyu, **Hao Yang**, *et. al.*, Bismuth oxyhydroxide-Pt inverse interface for enhanced methanol electrooxidation performance, *Nano Lett.,* 2020, **20**, 7751-7759.
24. **Hao Yang**, Tao Cheng, William A. Goddard III, *et. al*., Design of a one-dimensional stacked spin peierls system with room-temperature switching from quantum mechanical predictions, *J. Phys. Chem. Lett.*, 2019, **10**, 6432-6437.
23. Tingting Wang,[#] Miao Wang,[#] **Hao Yang**,[#] *et. al*., Weakening hydrogen adsorption on nickel via interstitial nitrogen doping promotes bifunctional hydrogen electrocatalysis in alkaline solution, *Energy Environ. Sci.*, 2019, **12**, 3522-3529. (Highlighted as front cover, [#]Co-First Author.)
22. Saber Naserifar, Julius J. Oppenheim, **Hao Yang**, *et. al.*, Accurate non-bonded potentials based on periodic quantum mechanics calculations for use in molecular simulations of materials and systems, *J. Chem. Phys.*, 2019, **151**, 154111.
21. Jin Qian, Yifan Ye, **Hao Yang**, *et. al*., Initial steps in forming the electrode-electrolyte interface: H_2O adsorption and complex formation on the

Ag(111) surface from combining quantum mechanics calculations and ambient pressure X-ray photoelectron spectroscopy, *J. Am. Chem. Soc.*, 2019, **141**, 6946-6954.

20. Yifan Ye,[#] **Hao Yang**,[#] Jin Qian,[#] *et. al.,* Dramatic differences in CO_2 adsorption and initial steps of reduction between Ag and Cu, *Nat. Comm.,* 2019, **10**, 1875. ([#]Co-First Author.)
19. He-Tuo Chen , **Hao Yang** , *et. al.,* Determining the quality factor of dielectric ceramic mixtures with dielectric constants in the microwave frequency range, *Sci. Rep.*, 2017, **7**, 14120.
18. Shao-Xian Liu, Chen Xue, **Hao Yang**, Xiao-Ming Ren, *et. al.*, Intercalated hybrid of kaolinite with KH_2PO_4 showing high ionic conductivity ($\sim 10^{-4}$ $S \cdot cm^{-1}$) at room temperature, *Solid State Sci.,* 2017, **74**, 95-100.
17. **Hao Yang**, Xiao-Ming Ren, *et. al.*, Insights into understanding water mediated proton conductivity in intercalated hybrid solid of kaolinite at ambient temperature, *New J. Chem.*, 2016, **40**, 10233-10239.
16. **Hao Yang**, Xiao-Ming Ren, *et. al.* Low-cost and environmental-friendly kaolinite-intercalated hybrid material showing fast formaldehyde adsorbing behavior, *ChemistrySelect*, 2016, **1**, 2181-2187.
15. Tian-Yu Chen, Lei Shi, **Hao Yang**, Xiao-Ming Ren, *et. al.*, Fabrication of a homogeneous, integrated, and compact film of organic-inorganic hybrid $Ni(en)_3Ag_2I_4$ with near-infrared absorbance and semiconducting features, *Inorg. Chem.,* 2016, **55**, 1230-1235.
14. **Hao Yang**, Xiao-Ming Ren, *et. al.*, Observation of a magnetic phase transition but absence of an electrical response in a new two-dimensional mixed-valence nickel-bis-dithiolene molecular crystal, *RSC Adv.*, 2015, **5**, 13857-13866.
13. Xiao-Pei Li,[#] **Hao Yang**,[#] Xiao-Ming Ren, *et. al.,* Investigation of the structure and ionic conductivity of intercalated kaolinites with potassium acetate in hydrous and anhydrous phases, *Dalton Trans*., 2015, **44**, 4665-4670. ([#]Co-First Author.)
12. Xiao-Qing Huang, **Hao Yang**, Xiao-Ming Ren, *et. al.,* Intercalation of lamellar

mineral kaolinite with 2-picolinic acid: facile preparation, crystal structure optimization, and proton conductivity, *Eur. J. Inorg. Chem.*, 2015, 4708-4714.

11. Xin Sun, **Hao Yang**, Xiao-Ming Ren, *et. al.,* Crystal structures, magnetic and electric properties of two new two-dimensional bis(2-thioxo-1, 3-dithiole-4, 5-dithiolato)nickelate complexes, *Syn. Met.*, 2015, **209**, 112-118.
10. **Hao Yang**, Xiao-Ming Ren, *et. al.,* Syntheses, crystal structures and magnetic properties of two halogen bridged dinuclear copper(II) complexes [(4, 4′-diethylester-2, 2′-biquinoline)$_2$Cu$_2$(μ-X)$_2$X$_2$] (X^- = Cl^-, Br^-), *Polyhedron*, 2014, **83**, 24-29. (Invited paper in special issue of 'Coordination Chemistry in China').
9. **Hao Yang**, Xiao-Ming Ren, *et. al.,* Experimental and theoretical investigation of magnetic and photoconductive natures for a novel two-dimensional mixed-valence bis(2-thioxo-1,3-dithiole-4,5-dithiolato)nickel- ate molecular solid, *Inorg. Chem. Front.*, 2014, **1**, 426-433.
8. Guo-Jun Yuan, **Hao Yang**, Xiao-Ming Ren, *et. al.,* Precisely tunable magnetic phase transition temperature through the formation of a molecular alloy in $[Ni_xPt_{1-x}(mnt)_2]^-$-based spin systems (mnt^{2-} = maleonitriledithiolate, x = 0.09-0.91), *Dalton Trans*., 2014, **43**, 11908-11914.
7. Qiao Qiao, **Hao Yang**, Xiao-Ming Ren, *et. al.,* Intercalated supramolecular compounds of kaolinite with ethanolamine and ethylene glycol: structures and dielectric properties, *Dalton Trans*., 2014, **43**, 5427-5434.
6. Xuan-Rong Chen, Wei-Hua Ning, **Hao Yang**, Xiao-Ming Ren, *et. al.,* Observation of hysteretic magnetic phase transitions coupled with orientation motion of ions and dielectric relaxation in a one-dimensional nickel-bis-dithiolene molecule solid, *Dalton Trans*., 2014, **43**, 6251-6261.
5. Wei-Hua Ning, Xuan-Rong Chen, **Hao Yang**, *et. al.,* Two segregated columnar stack platinumbis-dithiolene molecule solids showing spin-peierls-type transition above room temperature, *Dalton Trans*., 2014, **43**, 2997-3004.
4. Hai-Bao Duan, Xuan-Rong Chen, **Hao Yang**, Xiao-Ming Ren, *et. al.*, Disorder-order transformation and significant dislocation motion cooperating with a surprisingly large hysteretic magnetic transition in a nickel-bisdithiolene

spin system, *Inorg. Chem.,* 2013, **52**, 3870-3877.

3. Guang-Xiang Liu, Wei Guo, **Hao Yang**, *et. al.*, Synthesis, crystal structure, electronic absorption and magnetic properties of a novel anion-radical salt based on 7, 7, 8, 8-tetracyanoquinodimethane, *J. Chem. Crystallogr.*, 2011, **41**, 1262-1267.
2. Guang-Xiang Liu, **Hao Yang**, *et. al.*, Three new nickel(III) compounds based on 2-thioxo-1,3-dithiole-4,5-dithiolate: syntheses, structures, magnetic properties and theoretical analyses, *Polyhedron*, 2010, **29**, 2916-2923.
1. Guang-Xiang Liu, **Hao Yang**, *et. al.*, A trinuclear Cu(II) complex from the use of phenyl 2-pyridyl ketoxime: structure and magnetic behavior, *Synth. React. Inorg. M.*, 2010, **40**, 421-424.