Xiao-Li PEI

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Education

- 2010/9 – 2015/6: **Ph.D. in Physical Chemistry**

Xiamen University, Fujian, China
Thesis: Auration of C-H/N-H Bonds in Small-molecules with Oxo-Au(I)-Ag(I) Clusters
Thesis Advisor: Prof. Quan-Ming Wang

- 2006/9 – 2010/6: **B.S. in Applied Chemistry**

Huazhong Agricultural University, Wuhan, China
Thesis: Study on Synthesis and Biological Activity of N'-(2-methoxyphenyl)-N-nitro-N-(2,6-dibromo-4-fluorophenyl)urea
Thesis Advisor: Prof. Changshui Chen

- 2008/3 – 2010/6: **B.S. in Pharmacy** (Secondary Major)

Wuhan University, Wuhan, China
Thesis: Study on Preparation of Modified Pachymaran as Amphiphilic Molecules Nanometer Microballoons and Its Capability as Drug Carrier
Thesis Advisor: Assoc. Prof. Yuling Xiao

Current Position

- 2021/8 – now: Project Assistant Professor, Prof. Shionoya Laboratory, Department of Chemistry, Graduate School of Science, the University of Tokyo, Japan

Previous Positions

- 2019/5 – 2021/8: Postdoctoral Researcher, Prof. Shionoya Laboratory, Department of Chemistry, Graduate School of Science, the University of Tokyo, Japan
- 2016/9 – 2019/2: Postdoctoral Researcher, Prof. Echavarren Laboratory, Institute of Chemical Research of Catalonia (ICIQ), Spain
- 2016/1 – 2016/8: Research Assistant, State Key Laboratory of Physical Chemistry of Solid Surfaces, Xiamen University, Fujian, China
- 2015/7 – 2015/12: Civil Servant, Guigang Food and Drug Administration, Guangxi, China

Participation in Funded Project

- Polynuclear Gold Cluster Catalysis H2020-MSCA-IF-2016
  Host: Prof. Antonio M. Echavarren's Group, Institute of Chemical Research of Catalonia (ICIQ), Spain

Research Interests

1. Rational design and synthesis of ligand-protected homo-/hetero-coinage metallic clusters;
2. Single-crystal X-ray diffraction structural analysis;
3. Structure-property relationship studies of coinage metal clusters, including luminescence, chirality, and catalytic activities.

Attendance to Conferences

- **The 101st CSJ Annual Meeting**, March 19-22, 2021, online, Japan
  Oral Presentation: Chiral Twist in Gold(I) Octahedron Generating Asymmetric Carbon Centre
- **ICIQ-INTECAT School**, December 11-13, 2018, Tarragona, Spain
  Oral Presentation: From Mono- to Bi-metallic Catalysts: Anionic-Arylphosphines-Stabilized Small Gold and Gold-Silver Clusters
- **GOLD 2018**, July 15-18, 2018, Paris, France
  Oral Presentation: Anionic-Arylphosphines-Stabilized Small Gold and Gold-Silver Clusters: From Mono- to Bi-metallic Catalysts
- **XVI Biennial Meeting - Spanish Royal Society of Chemistry (RSEQ)**, June 25-29, 2017, Sitges, Spain
  Poster: Silver Doping in Hexanuclear Gold(I) Clusters Stabilized by Hemilabile Phosphine

Publications

1. **X.-L. Pei**, Y. Yang, Z. Lei, Q.-M. Wang. Geminal Tetraauration of Acetonitrile: Hemilabile-Phosphine-Stabilized Au_8Ag_4 Cluster Compounds. ***J. Am. Chem. Soc.*** **2013**, *135*, 6435–6437.
2. Y. Yang, **X.-L. Pei**, Q.-M. Wang. Postclustering Dynamic Covalent Modification for Chirality Control and Chiral Sensing. ***J. Am. Chem. Soc.*** **2013**, *135*, 16184–16191.
3. Z. Lei, **X.-L. Pei**, Z. G. Jiang, Q.-M. Wang. Cluster Linker Approach: Preparation of a Luminescent Porous Framework with NbO Topology by Linking Silver Ions with Gold(I) Clusters. ***Angew. Chem., Int. Ed.*** **2014**, *53*, 12771–12775. *(Inside Back Cover.)*
4. **X.-L. Pei**, Y. Yang, Z. Lei, S.-S. Chang, Z.-J. Guan, X.-K. Wan, T.-B. Wen, Q.-M. Wang. Highly Active Gold(I)-Silver(I) Oxo Cluster Activating sp^3 C-H Bonds of Methyl Ketones under Mild Conditions. ***J. Am. Chem. Soc.*** **2015**, *137*, 5520–5525.
5. Y. Yang, J.-H. Jia, **X.-L. Pei**, H. Zheng, Z.-A. Nan, Q.-M. Wang. Diastereoselective Synthesis of *O* Symmetric Heterometallic Cubic Cages**.** ***Chem. Commun.*** **2015**, *51*, 3804–3807.
6. Z. Lei, Z.-J. Guan, **X.-L. Pei**, S.-F. Yuan, X.-K. Wan, J.-Y. Zhang, Q.-M. Wang. Atomic Precise $Au_{10}Ag_2$ Nanocluster with Red-NIR Dual Emission. ***Chem. Eur. J.*** **2016**, *22*, 11156–11160.
7. Z. Lei, **X.-L. Pei**, Z.-J. Guan, Q.-M. Wang. Full Protection of Intensely Luminescent Gold(I)-Silver(I) Cluster by Phosphine Ligands and Inorganic Anions. ***Angew. Chem., Int. Ed.*** **2017**, *12*, 7117–7120. *(Hot paper, Inside Back Cover.)*
8. C. García-Morales, **X.-L. Pei,** J. M. Sarria Toro, A. M. Echavarren. Direct Observation of Aryl Gold(I) Carbenes that Undergo Cyclopropanation, C−H Insertion, and Dimerization Reactions. ***Angew. Chem., Int. Ed.*** **2019**, *58*, 3957–3961.
9. **X.-L. Pei**, A. Pereira, E. S. Smirnova, A. M. Echavarren. Small Gold(I) and Gold(I)-Silver(I) Clusters via C-Si Auration. ***Chem. Eur. J.*** **2020**, *26*, 7309–7313.
10. Z. Lei, **X.-L. Pei**, H. Ube, M. Shionoya. Reconstituting the C-Centered Hexagold(I) Clusters with N-Heterocyclic Carbene Ligands. ***Bull. Chem. Soc. Jpn.*** **2021**, doi:

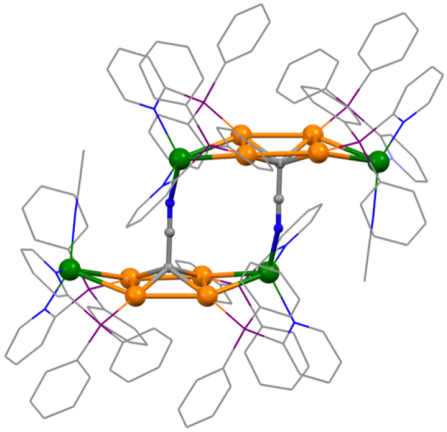
10.1246/bcsj.20210060. *(Inside Back Cover.)*

11. **X.-L. Pei**, Z.-J. Guan, Z.-A. Nan, Q.-M. Wang. Heterometallic Coinage Metal Acetylenediide Clusters Showing Tailored Thermochromic Luminescence. *(Hot paper)* ***Angew. Chem., Int. Ed.*** **2021**, *60*, 14381–14384.

Research Summary

1. Activation of C(sp^3)-H bond in small organic molecules with the oxonium gold-silver clusters stabilized by hemilabile-phosphines.

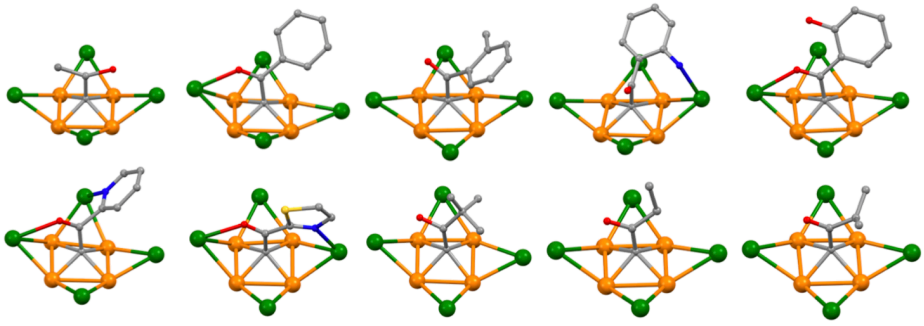
a) Germinal Tetraauration of Acetonitrile: Hemilabile-Phosphine-Stabilized Au_8Ag_4 Cluster Compounds. (*J. Am. Chem. Soc.* **2013**, *135*, 6435–6437.)



We discovered that oxonium gold(I)-silver(I) clusters can fully deprotonate acetonitrile at room temperature, leading to unprecedented tetra-auration of acetonitrile with the assistance of a protic solvent. The crystal structures was determined by X-ray crystallography diffraction. A concerted metalation/deprotonation process for the C−H activation of acetonitrile was proposed, indicating that the oxo ion plays a key role in the C−H activation of acetonitrile, and this provides new insight in terms of the involvement of Ag_2O in gold-catalyzed processes.

b) Highly Active Gold(I)-Silver(I) Oxo Cluster Activating sp^3 C-H Bonds of Methyl Ketones under Mild Conditions. (*J. Am. Chem. Soc.* **2015**, *137*, 5520–5525.)

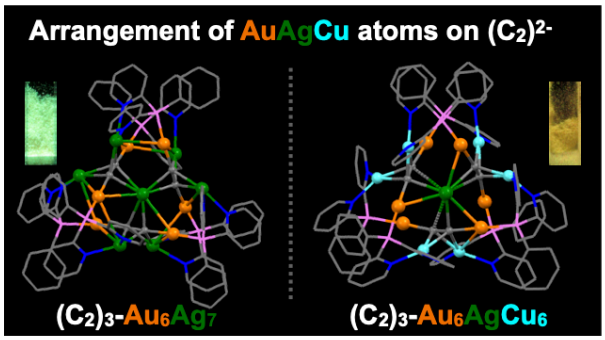
A highly active oxo-gold(I)-silver(I) cluster with hemilabile phosphine ligands, *i.e.* $[OAu_3Ag_3(PPhpy_2)_3](BF_4)_4$, can activate C($sp^3$)-H bonds under mild conditions for a broad scope of methyl ketones, leading to the isolation of heterometallic Au(I)−Ag(I) clusters $RCOCAu_4Ag_4(PPhpy_2)_4(BF_4)_5$ ($PPhpy_2$ = bis(2-pyridyl)phenylphosphine). The scope displayed an interesting selectivity of activation: C-H bonds in $–COCH_3$ rather than N–H bond in $–NH_2$ or O−H bond in –OH, and the terminal methyl group is preferred over secondary or tertiary sp^3 C−H bonds. This work highlights the powerful reactivity of metal clusters toward C−H activation and sheds new light on gold(I)-mediated catalysis.



2. Strategy to access multifunctional heterometallic coinage metal clusters by using hemilabile-phosphines-protected oxonium gold-silver clusters as synthetic precursor.

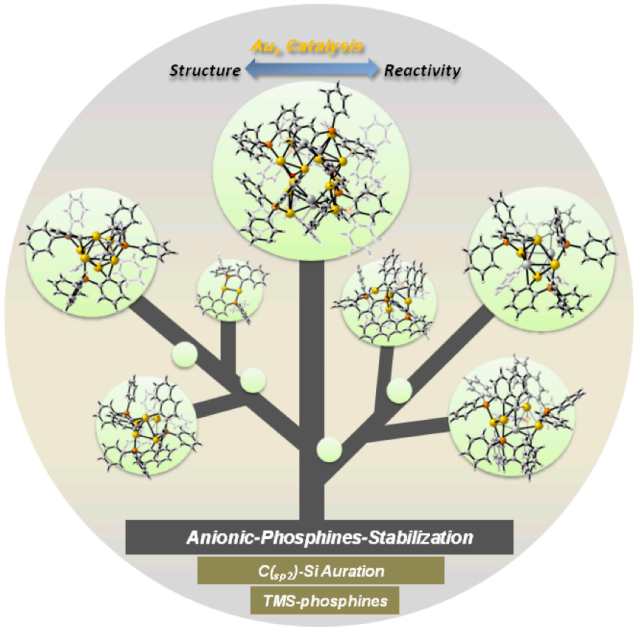
Heterometallic Coinage Metal Acetylenediide Clusters Showing Tailored Thermochromic Luminescence. (*Angew. Chem., Int. Ed.* **2021**, *60*, 14381–14384.)

We found the hemilabile-phosphine-supported heterometallic cluster $[O(AuL)_3Ag](BF_4)_2$ (L = phenylbis(2-pyridyl)phosphine ($PPhpy_2$)) is a also useful synthetic precursor. The replacement of O^{2-} with C_2^{2-} promotes the formation of the heterometallic coinage metal acetylenediide clusters, $[(AuL)_6Ag_7(C{\equiv}C)_3](BF_4)_7$ and $[(AuL)_6AgCu_6(C{\equiv}C)_3](BF_4)_7$. They are the first examples of bimetallic and trimetallic coinage metal acetylenediide clusters. They are isostructural but display different thermochromic luminescence. The replacement of silver with copper changes the HOMO character to induce dual-emission in $(C_2)_3$-Au_6AgCu_6, and this dual-emission is associated from two emissive states favored at different temperatures.



3. Protocols of auration of C-Si bond (Au/Si transmetalation) to achieve gold and gold-silver clusters as catalysts for the gold-catalyzed cycloisomerization of enyes under homogeneous conditions. (*Chem. Eur. J.* **2020**, *26*, 7309–7313.)

Auration of *O*-trimethylsilyl arylphosphines led to the formation of gold and gold-silver clusters with ortho-metallated phosphines displaying 3c-2e Au-C-M bonds (M = Au/Ag). Hexagold clusters $[Au_6L_4](X)_2$ were obtained by reaction of (L-TMS)AuCl with AgX, whereas reaction with AgX and Ag_2O leads to gold-silver clusters $[Au_4Ag_2L_4](X)_2$. Oxo-trigold(I) species $[Au_3O]^+$ were identified as the intermediates in the formation of the silver-doped clusters. Other $[Au_5]$, $[Au_4Ag]$, and $[Au_{12}Ag_4]$ clusters were also obtained. Clusters containing PAu-Au-AuP structural motif displayed good catalytic activities in the activation of alkynes under homogeneous conditions.



Therefore, my previous studies focused on the gold(I) and gold(I)-silver(I) clusters with phosphine ligands, illustrating their unique structures, the reactivity of C-H bond activation, luminescent properties, and further investigation in gold-catalyzed homogeneous catalysis with gold cluster-based catalysts. These results not only demonstrate the strategies on the construction of gold and gold-silver clusters with various phosphine ligands, but also give deep insights into the mechanistic understanding of sp^3 C-H bond activation, and the potential application for gold-catalyzed transformations.