

## Yachao Su

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### EDUCATION AND TRAINING

01/10/2016 – 30/06/2020 Xiangtan, China BACHELOR Xiangtan University

Website https://www.xtu.edu.cn/ | Field of study Polymer Materials and Engineering | Final grade 3 |

Thesis Preparation of Nanocomposites with High Dielectric and Low Loss

01/10/2021 – 30/06/2024 Xiangtan, China **MASTER** Xiangtan University

# 1.The Influence of Ligand Structural Variations on the Stability and Other Properties of Monolayer-Protected Gold Clusters

### 2.Study of the Catalytic Properties of Gold Nanoclusters under the Influence of Different Ligands

Website https://www.xtu.edu.cn/ | Field of study Physical Chemistry | Final grade 3 |

**Thesis** The influence of different types of thiol ligands at the interface on the geometric structure, stability, and catalytic performance of gold nanoclusters.

01/10/2024 – 30/09/2027 Paris, France DOCTORAL STUDENT Chimie ParisTech - PSL

The conception of new white emitting single molecule materials is challenging from a purely experimental perspective and insights on the complex photophysical behavior from a theoretical point of view are highly valuable for their design. From a theoretical perspective, these materials are a perfect playground to test the ability of novel approaches for describing excited states of different nature and their modulation due to the presence of a crystalline environment. Indeed, to correctly predict dual emission from a single molecule one needs to develop and interface efficient methods enabling to compute 1) the structure and energetic of excited states of different characters (locally excited, intra or inter molecular charge transfer, excimeric) and 2) the effect of the crystalline matrix on them.

The aim of the present project is to setup computational protocols based on Density Functional methods that will enable to describe and predict emission of organic compounds in light of their use as single molecule white emitting materials and to predict the link between the macroscopic emission behavior of the molecular material and their chemical structure from first principles.

Website <a href="https://www.chimieparistech.psl.eu/">https://www.chimieparistech.psl.eu/</a> | Field of study Chemistry

Thesis Modelling white light emitting materials using Density Functional based approaches

### PUBLICATIONS

2023

<u>Ultra-long cycle life organic-sodium batteries enabled by thiophene-based porphyrin in-situ</u> <u>electropolymerization.</u>

Zeng, Youlian, et al. Chemical Engineering Journal 453 (2023): 139951.

2023

A bipolar porphyrin molecule for stable dual-ion symmetric batteries with high potential.

Zeng, Youlian, et al. Chemical Communications 59.33 (2023): 4962-4965.