Francesc Penas Hidalgo
Master in Synthesis, Catalysis and
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RESEARCH INTERESTS

Theoretical and computational chemistry

- Static DFT calculations
- Clasical Dynamics
- Microkinetic models
- Python
- Periodic systems calculations
- Other interesting methodologies

SUMMARY

During my bachelor and master, I have worked on polyoxometalates. I have experience in this systems predicting theoretically and computationally their properties in homogeneous catalysis. My objective is to understand the role of polyoxometalates in the homogeneous catalytic reduction of CO2 and explore other systems like frustrated Lewis pairs to do the same task. I also aimed to explore metal-organic frameworks to catalyse heterogeneously the same reaction involving and learning new methodologies unknown for me yet.