Institute of Theoretical and Computational Chemistry

One post-doc position

Duration: 24 months

Salary: 30-35 k€/year depending on proven expertise

Project: Atom-Dispersed Catalysts for the Thermo-Photo Valorization of CO_2
Funding: Spanish AEI AD-TPCO$_2$ project
Task: Computational Modeling

Advisors:

Prof. Dr. Francesc Illas (francesc.illas@ub.edu)
Prof. Francesc Viñes (francesc.vines@ub.edu)

Context: Within the AD-TPCO2 project we will study the valorization of CO_2 greenhouse gas through possible thermo-photocatalytic processes for its conversion towards fuels (CH_4 and CH_3OH) or fuel precursors (CO for Fischer-Tropsch) using novel and rationale-designed multication/anion oxide catalysts, with the ultimate goal of engineering and optimizing the solar light visible light absorption, either near-UV or near-IR, while effectively using the excited states to trigger the chemical conversion of CO_2 on the aforementioned chemical products. This will be carried out with intertwined experimental and theoretical research, which constant feed-back. The objective of AD-TPCO$_2$ is to provide develop new and suited thermo-photocatalysts for CO_2 utilization and valorization, helping at closing the C-cycle in a sustainable fashion while opening new chemical conversions of industrial, technologic, and economic interest to convert CO_2 economy into a waste-to-product model, thus helping at mitigating climate change.

Project: The computational research will be conducted at the Computational Materials Science Laboratory (CMSL)[1] of the University of Barcelona (UB),[2] a group member of the Institute of Theoretical and Computational Chemistry (IQTC)[3] of the UB, a recognized excellence María de Maeztu research unit, a distinction label provided by the Spanish research agency (AEI) in a highly competitive basis. The study will involve studying (co-)doping of oxide-based slab and nanoparticle models, analysis of the electronic structure at ground and excited states, to evaluate reaction profiles on ground and excited states, and to support the experimental team lead by Prof. Marcos Fernández

García at the Institute of Catalysis and Petrochemistry (ICP)[4] in the interpretation of catalyst identification by standard techniques such as IR, XPS, XAS or XRD. The computational part will include modeling, DFT optimizations, location of transition states, kinetic analysis based on transition state theory and ab initio thermodynamics, and IR and core level binding energies estimations. The study will include high-throughput computation and analysis by set-up machine learning tools.

Candidates: Required qualifications include a solid background in Chemistry, Physics, or Chemical Engineering or similar, with emphasis on Physical Chemistry, Catalysis, and Theoretical and Computational Chemistry. Knowledge and experience in modern coding languages (bash scripting, python, atomic simulation environment - ASE) are beneficial. Knowledge and experience on VASP and/or FHI-AIMS codes are also beneficial. Very good communication skills in English and ability to produce acceptable drafts and scientific reports are a must. Spanish and/or Catalan language skills will be considered.

Location: The CMSL offices are located within the Chemistry Faculty of the UB, one of the oldest Universities in Spain, with more than 5 centuries of existence and ranked #1 in Spain in the Shanghai and other international rankings. Aside, UB is located within the beautiful city of Barcelona, Spain, known by its gastronomy, culture, modernist architecture, and nice weather. The Chemistry Faculty is found within the Barcelona Knowledge Campus, an exciting scientific and international environment. In addition, the collaboration with the ICP will require the occasional visit to their facilities in Madrid, capital of Spain, a renowned historical city, with its own culture, gastronomy, and with highly famous museums.

Application: We are looking forward to receiving your email application including a letter of motivation (one page), a short CV (two pages), and contact details of two referees. The email must be addressed to francesc.illas@ub.edu and francesc.vines@ub.edu containing “AD-TPCO2 Postdoc position” in the title.

References:

[1] https://sites.google.com/view/cmsl-research-barcelona/home?authuser=1
[2] https://www.ub.edu
[3] https://www.iqtc.ub.edu
[4] https://icp.csic.es/es/