1 PhD position on: « Bimetallic catalyst knowledge-based development for energy applications » at Italian CNR

Location: National Research Council (CNR), Pisa (Tuscany), Italy
Time frame: Start before October 1st 2020 – 2.5 year term, PhD curriculum
Deadline for applications: May 31st 2020

1 PhD position is available funded by a EU ITN project: "Bimetallic catalyst knowledge-based development for energy applications" (acronym: BIKE) within the call: H2020-MSCA-ITN-2018. The positions will be held at CNR in Pisa, Italy (supervisor: Dr. Alessandro Fortunelli) – theory work will be conducted in close collaboration with DTU, Denmark (Profs. Tejs Vegge and Heine A. Hansen) and with experimental partners. The topic is the computational predictive modeling and design of bimetallic catalysts for energy management, in particular for blue and green hydrogen production via Aqueous Phase Reforming of Liquid Renewable Feedstocks. Other beneficiaries of the ITN are academia and research centers: Italian CNR, Technical University of Catalonia (Spain), CSIC (Spain), BAS (Bulgaria), Durham University, UK), KIT (Germany), NTU (Norway), and two companies: Johnson Matthey (UK) and ICI CALDAIE SPA (Italy).

- **Scientific context**

The MSCA-ITN-ETN (European Training Network) project BIKE[1] is a network for training of 14 early stage researchers (ESRs), who will develop and apply, by an innovative "holistic" approach, the next generation of bimetallic catalysts for hydrogen production via a synergy among predictive modelling, advanced characterization, knowledge-based design and novel preparation of catalysts, and explorative testing. The goal of the theory ESR at CNR is to learn, develop and apply hierarchical multi-scale simulation protocols for accurate modeling of heterogeneous nano-catalysis under realistic operating conditions of temperature and coverage, so as to provide information, insight and design of bimetallic catalysts for aqueous phase reforming of liquid renewable feedstocks. PhD curriculum will be held at Pisa University.

- **Related Publications :**
  - Q. An, Y. Shen, A. Fortunelli, W. A. Goddard, QM-Mechanism-Based Hierarchical High-Throughput in Silico Screening Catalyst Design for Ammonia Synthesis. *J. Am. Chem. Soc.* (2018) **140**, 17702–17710, DOI: 10.1021/jacs.8b10499
  - T. Cheng, A. Fortunelli, W. A: Goddard "Reaction intermediates during *operando* electrocatalysis identified from full solvent quantum-mechanics molecular dynamics" *Proc. Nat. Ac. Sci.* (2019) **116**, 7718-7722, DOI: 10.1073/pnas.1821709116.

We are looking for a motivated graduate student/early-stage researcher, with interest and knowledge in predictive modeling of catalysis. Expertise in density-functional theory (DFT) for structure and electronic band structure prediction is a pre-requisite, experience in reactive simulations is a plus. Salary will be granted for 30 months, although PhD curriculum lasts 3 years (starting immediately after successful interview). The candidate must have been awarded a Master Degree in Chemistry or Physics or Materials Science since no longer than July 2016, and not have resided in Italy for more than 12 out of the last 36 months. Queries may be sent via email to:

Scientific supervisor: Alessandro Fortunelli, CNR, Pisa, Italy[2]
Contacts: Alessandro Fortunelli, e-mail : alessandro.fortunelli@cnr.it

[1] https://cordis.europa.eu/project/rcn/218448/en, https://www.bike-msca.eu/
[2] http://www.researchgate.net/profile/Alessandro_Fortunelli/, http://www.pi.iccom.cnr.it/ThC2-Lab