3 PhD positions on: « Bimetallic catalyst knowledge-based development for energy applications » at CNR and DTU

2 Locations: National Research Council (CNR), Pisa (Tuscany), Italy
& Danish Technical University (DTU), Lyngby (Copenaghen), Denmark
Time frame: Start around November 2019 – 3 year term, PhD curriculum

3 PhD positions are available funded by a recently approved EU ITN project: "Bimetallic catalyst knowledge-based development for energy applications" (acronym: BIKE) within the call: H2020-MSCA-ITN-2018. 2 positions will be held at CNR in Pisa, Italy (supervisor: Dr. Alessandro Fortunelli) and 1 position at DTU, Lyngby, Denmark (supervisors: Prof. Tejs Vegge and Prof. Heine A. Hansen) – thery work will be conducted in close collaboration between the 2 institutions. The topic is the computational predictive modeling and design of bimetallic catalysts for energy management, in particular for blue and green hydrogen production processes. Other beneficiaries of the ITN conducting experimental work 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 3 theory ESRs at CNR and DTU is to learn, develop and apply hierarchical multi-scale simulation protocols for accurate modelling of heterogeneous nano-catalysis under realistic operating conditions of temperature and coverage, so as to provide information, insight and design of bimetallic catalysts for CH4 steam reforming, aqueous phase reforming, and water electrolysis.

- **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
  - Steen Lysgaard, Paul C. Jennings, Jens Strabo Hummelshøj, Thomas Bligaard, Tejs Vegge, Machine Learning Accelerated Genetic Algorithms for Computational Materials Search, DOI: 10.26434/chemrxiv.7411172.v2 (2018).

We are looking for 3 motivated graduate students/early-stage researchers, with interest and knowledge in predictive modeling of catalysis. Expertise in density-functional theory (DFT) for structure and electronic band structure prediction and reactive simulations is a pre-requisite. Official calls adhering to EU recruiting procedures (including stipends) will soon follow. In the meantime, pre-applications (including reference persons) can be sent to either CNR or DTU via email to:

Scientific supervisors: Alessandro Fortunelli, CNR, Pisa, Italy[2]
Tejs Vegge & Heine A. Hansen, DTU, Lyngby, Denmark[3]

Contacts: Alessandro Fortunelli, e-mail : alessandro.fortunelli@cnr.it
Tejs Vegge, e-mail : teve@dtu.dk
Heine A. Hansen, e-mail : heih@dtu.dk

[1] https://cordis.europa.eu/project/rcn/218448/en
[2] http://www.researchgate.net/profile/Alessandro_Fortunelli/, http://www.pi.iccom.cnr.it/ThC2-Lab
[3] https://www.dtu.dk/english/service/phonebook/person?id=5334&tab=1