

NOMAD Laboratory Centre of Excellence

Industry Interview - Dr. Ansgar Schäfer (BASF)

BASF are the largest chemical producer in the world, so it comes as no surprise that their wish list for the *NOMAD Laboratory CoE* is mainly catalysis-centred. In fact, BASF expressed the hope that the CoE will be able to leverage state of the art computational tools to speed up the discovery and development of novel catalytic materials. This is of paramount importance for a company like BASF, since even a minimal selectivity improvement for a production process can translate into savings worth millions/year in raw materials, improved carbon footprint and process yield, etc. In this context, Quantum Mechanical (QM) simulations have the potential to analyse even complex reaction mechanisms, possibly identifying limiting steps and helping to plan further developments in a more informed way.

Dr. Schäfer identified some **high level concepts** that the *NOMAD Laboratory CoE* should address:

- The search space should (ideally) be made as comprehensive as possible to cover all known materials.
- Suitable metrics/descriptors should be sought to efficiently navigate a given search space, such as:
 - o Classification of materials (selection/exclusion),
 - o Identification and exploitation of similarities,
 - o Identification of unexplored areas (white spots).
- Generate understanding: why is this materials working/not working?
- Provide design principles to drive development.
- If possible, construct a workflow for addressing real-world catalysis challenges.

Specific requests from BASF included:

- Provide both bulk and surface structures and properties (or seek a link between the two).
- Provide structures and properties for materials under real-world state conditions:
 - o Medium to high temperature, thermal stability, phase equilibria,
 - o Gas phase, adsorption equilibria.
- Provide a feedback loop between simulations and experiments to aid model refinement.
- Facilitate combination of in-house and NOMAD data (keeping in mind intellectual property issues).
- Provide an infrastructure from which it is possible to easily trigger a new calculation when/if needed.

<http://nomad-coe.eu/>

@NoMaDCoE

www.facebook.com/nomadCoE



UNIVERSITAT DE
BARCELONA



Pintail



This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 676580. The materials presented and views expressed here are the responsibility of the author(s) only. The EU Commission takes no responsibility for any use made of the information set out.