DEFNET-641887 MSCA-ITN-2014-ETN Horizon 2020

Individual Training and Supervision Plans (ITSP)

Year-1

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Brief overview of research project and major accomplishments expected (half page):

The key objective of the research project is to understand the structure, probability of formation and the reactivity of defects in Metal-Organic Frameworks (MOFs) on an atomistic level by computational multiscale simulation methods. This involves both defects occurring in regular bulk material, like missing linker defects, or local structural deviations due to the use of defect-linkers added on purpose (engineered defects). The reactivity of defects concerns primarily catalytic reactions.

This objective will be achieved by the use of first principles derived force fields (MOF-FF) developed at the RUB. A consistently embedded QM/MM method (QM level of theory equal to FF parametrization) for modelling the electronic structure of local defects will be developed, allowing the prediction of oxidation states and the coordination environment, as well as the determination of reactive intermediates in catalytic processes. A computation of spectroscopic signatures (e.g. vibrational modes) establishes a link to the experimental data and to validate the theoretical predictions. On the basis of the QM/MM calculations, a parametrization of a defect force field, that allows to describe the defect also on the FF level, will be attempted. By "alchemical" transformations free energies of different defects, and thus the probability of their formation will be determined. A long term goal will be the study of collective defects and correlation between defects, which implies mesoscale simulations. To arrive at this length scale, "coarse-grained" force field models will be used.

Project Title: ***Theoretical prediction of molecular and electronic structure of defects in MOFs***

Work-package: WP3

Planned secondments:

- Software for Chemistry & Materials / Scientific Computing & Modelling (SCM) @ Amsterdam, The Netherlands;
- Center for Molecular Modeling (CMM) @ Ghent, Belgium;
- Other beneficiaries and/or partner organizations in order to support the experimental characterization.

Long term career goals and objectives (over 3 years)

1. **Goals & Objectives:**
   Our goals are 1-to understand the deepest nature of interactions of defects in defective Metal-Organic Frameworks (DEMOFs) and the resulting phenomena; 2-to simulate, support and predict experimental data; 3-to suggest reasonable tools for the design of DEMOF.
   The modelling of DEMOFs via Molecular Mechanics (MM) simulations shows several advantages against a simple Quantum Mechanics (QM) approach. Given that MM is generally less resource-consuming than QM, the phase space (positions and momenta) can be sampled more extensively, granting the investigation of higher structural complexity and longer disorder correlations even among different kinds of defect.
   Furthermore, the broader the computed distances and cell are, the more the spurious periodic effects that could mislead data interpretation of defects are prevented in a periodic boundary condition (PBC) fashion. Finally, the MM transferability is rather easier to be achieved, a highly demanded property where defects are wanted to change as desired. (defects themselves can be interpreted as local modifications of the crystalline structure)
   Some assumption must be done on a guessed structure, for example by the means of a single (even QM optimized) structure. Then, force fields (FFs) are tailored to accordingly reproduce an expected set of chemical/physical properties at the given accuracy.
   Where rationalizing particular properties with a FF provokes in any degree a lack of generality, a solution could be confining the QM calculations in the surroundings of a (somehow arbitrary, but strictly defect-related) reactive site, where accurate predictions are required, and extend the MM computation elsewhere. This hybrid approach, known as QM/MM (Quantum Mechanics/Molecular Mechanics), carries both the QM accuracy and MM speed out. The method incurred intensive study in biosimulations but, surprisingly, it has been developed only for a while in the case of DEMOFs.

2. **Do you have a clear and defined plan for your project ? What further research activity or other training is needed to attain these goals? For each goal, specify any areas where you feel you need additional training ? (include any techniques/instrumentations/ you want to learn ? scientific collaboration etc..)**
   - *Plan: "Advanced multiscale computational simulation methods for static properties (structure) of DEFNET materials. To support*

WP1 + WP2 by experimental data interpretation & predictions." (GA, Annex 1, p.17)

- The collaboration with institutes and ESRs involved in the same WP will be improved, and the benchmarking with other WPs besides.
- Insights about the taxonomy of existing FFs are mandatory, in particular reactive FFs and polarizable FFs.

Short Term objectives (1 year)

1. **Research results**
   - **Anticipated publications:**
     1. No anticipated publication in the short term
   - **Anticipated conference, workshop attendance, courses, and /or seminar presentations:**
     1. DEFNET Workshop @ UGent, Ghent, Belgium
        - Poster presentation
        - Hands-on session
     2. DEFNET School @ CSIC ITQ, Valencia, Spain
     3. CAMD Summer School @ DTU, Kgs. Lyngby, Denmark
     4. PISACMS Summer School @ UPCM, Paris, France
        - Poster presentation
     5. International MOF Conference @ Long Beach, California, USA
        - Poster presentation

2. **Research skills and techniques:**
   - **Training in specific new areas, or technical expertise/instrumentation etc:**
     1. **Specific new areas:**
        - Effective Fragment Potential (EFP)
        - Free energy calculation via non-physical (*alchemical*) pathways
        - Machine learning: evolutionary algorithms and supervised methods (semester course, 4 hours a week)
     2. **Technical expertise:**
        - Automated code review softwares
        - Debuggers and profilers
        - Static and dynamic program analysis

3. **Research management:**
    - **Fellowship or other funding applications planned (indicate name of award if known; include fellowships with entire funding periods, grants written/applied for/received, professional society presentation awards or travel awards, etc.)**
        1. No short-term funding planned

4. **Communication skills (Scientific presentation, Scientific communication):**
    - RUB Research School workshops
        1. "Paper writing: expert input to advance your papers and to develop a publication strategy" (one full-day workshop)
        2. "Optimizing writing strategies for publishing research" (three full-day workshop)
        3. Further workshops could be planned
    - Department of German as Foreign Language
        1. note that, even if the subject is English, the language of some RUB Research School communication workshop I'll intend to follow is German.
        2. Learning German, also, will help mentoring undergraduate students and supervising their thesis. (see "Other professional training")
        3. Lastly, several fundamental courses for scientists (History and Philosophy of Science, Logic, Epistemology) are German courses.

5. **Other professional training (course work, teaching activity):**
    - Assistance to side activities for undergraduate Chemistry courses (e.g. one week of lab support)
    - Tutoring undergraduated students (as a Tutor and Assistant in the Lecture "Scientific Programming Methods for Chemists")

6. **Anticipated networking opportunities:**
    - Apart from the DEFNET coordinated activities, the understanding of methodological and developing approach, as well as software project managing of other research groups, will be fruitful.

7. **Other activities with professional relevance (participation in group seminars, research colloquia, guest lectures, workshops) at the host institute:**
   - o CMC Group Seminar, weekly
   - o General Group Seminar, twice a week / weekly
   - o Guest lectures, monthly

Signature of ESR:
Date/Place

Signature of the Principle Supervisor (PS):
Date/Place

Signature of the Associated Supervisor (AS):
Date/Place

Prof. V. Van Speybroeck
12/09/2016

Signature of the Mentor (ME):
Date/Place