

## SPP 2080 Workshop for Ph.D. Students and Postdocs

Organized in conjunction with the DFG Priority Programme "SPP 2080"  
Leipzig, February 18-20, 2020

After the SPP2080 Status Meeting the 2<sup>nd</sup> SPP2080 PhD and PostDoc Workshop took place from 18<sup>th</sup> to 20<sup>th</sup> of February at Leipzig University. After a successful 1<sup>st</sup> workshop in September 2019 the focus of this workshop was a hands-on modelling and simulation course. Most PhDs and PostDocs within the SPP2080 have a background in chemistry and not chemical engineering. Therefore, not everybody has a background knowledge in modelling and simulation of chemical processes. However, this is important in the field of heterogeneous catalysis as length scales from the active site (<nm-nm) up to the reactor scale (cm-m) are relevant for the design of heterogeneous catalyzed chemical processes and a background knowledge is necessary for cooperation between chemists and chemical engineers. The topics of the workshops were: (i) a basic understanding of the Matlab software commonly used for simulations and modelling, (ii) the calculation of the thermodynamic equilibrium for the example reaction of the oxidative dehydrogenation of ethane to ethylene, (iii) the modelling of a continuously stirred tank reactor (CSTR) for the reaction under polytropic, isothermal and adiabatic conditions and (iv) the simulation of the start-up behavior of an isothermal plug flow reactor (PFR). The hands-on courses always consisted of a short introduction lecture followed by exercises with Matlab. The special thing about the course was that three chemical engineering PhD students from within the SPP2080 prepared and held the course. All participants could get a broad insight into the daily work of chemical engineers and based on this knowledge a better understanding for modelling and simulation was achieved. The existing collaborations between chemists and engineers within the SPP2080 are thus strengthen while new collaboration opportunities were fostered.

The second part of the PhD and PostDoc workshop was a course focused on scientific writing held by Greta Heydenrych from Wiley-VCH (Chief-editor of ChemPhysChem, ChemElectroChem, ChemPhotChem, Batteries&Supercaps and ChemSystemsChem). The course focused on different aspects of scientific publishing. First an introduction was given about the work of an editor and a publisher in general. This was followed by an explanation about the peer-review process and important steps of it. The participants received hints how to prepare a successful manuscript, the importance of the cover letter for the paper submission and some general guidelines were to submit their article. Furthermore, possible problematic point during the peer-review process were explained and how to deal with them. This consisted of tips how to deal with critical reviews, but also gave an insight to the PhDs and PostDocs how to prepare well revisions. Another topic which was highlighted was the initiative to increase open access publications, while this part was also composed of why publishers need to make money and how they invest the money in order to increase scientific outreach. These investments consist of licenses for DOI or ISSN numbers, support of databases, support of low-cost access to scientific journals in less developed countries, and many more. Furthermore, the role of ethics was discussed and the consequences of insulting the publisher's ethics guidelines were shown. All in all the scientific writing course was strongly interactive and the PhDs and PostDocs had many opportunities to ask questions and discuss with the speaker.

The scientific courses were complemented by a barbecue and general discussion about the planned summer school of the SPP2080. The PhD and PostDoc workshop was a great

opportunity for all participants to network and find potential support for their projects within the SPP2080. As the topic of the SPP2080 are dynamics in catalysis, this is also true for all the engaged PhDs and PostDocs who are really engaged in exchanging and sharing their knowledge with the others.

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*Participants of the 2nd PhD and PostDoc Workshop of the SPP2080 from 18<sup>th</sup> to 20<sup>th</sup> February at Leipzig University, Photo Credit: Erisa Saraci*