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Thesis Project Offer

Joint Research and Education Programme "Palestinian-German Science Bridge PGSB"
Forschungszentrum Jülich GmbH & Palestine Academy for Science and Technology

Thesis type*

☐ BSc	⊕ **MSc**	☐ PhD	Intended starting date (approx.):

Contact details of supervisor/responsible host at Forschungszentrum Jülich

Title*	Degree	First name*	Surname*
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Function*	Institute and homepage of institute*
Project Leader Theory and Modeling	IEK-4, http://www.fz-juelich.de/fusion

University affiliation in Germany*

Ruhr-University Bochum

Co-Supervisor at Palestinian university (if applicable)

Title	Degree	First name	Surname
Title	Degree		

Phone	E-mail

University/institution	Department/faculty/institute

Project description*

Implementation of model catalysts in a reaction network combining gas phase and surface reactions

Over the past decades there has been growing interest in plasma assisted CO2 conversion. This technology is based on the use of non-thermal plasmas for dissociation of CO2 and the production of syngas. The syngas, in turn, can be further processed into valuable fuels and chemicals. Moreover, combining a plasma with a catalyst has been proven to significantly increase the efficiency of the CO2 conversion process. However, these processes, especially the heterogeneous catalysis, are not completely understood. So, to take advantage of this undeniably good technology, it is necessary to investigate very fundamental processes in the plasma and at the plasma-catalyst interface. At IEK-4 numerical tools have been developed which allow the analysis of CO2 conversion in the gas phase with/without a catalyst. The underlying models are based on reaction kinetics which is a natural starting point to identify fundamental processes in a complex system where many reactions appear simultaneously. On the one hand the tools cover the simulation of reactions for a given set of reaction coefficients. On the other hand model discovery tools will be applied to data from plasma experiments (concentrations of different gas species and coverage of catalyst surfaces) to obtain the rate coefficients which form the concrete reaction kinetics model. For most experimental situations to be studied in the future the mathematical model is not known a priori. Then a sparse regression method is used to identify the best fit among several reasonable models, i.e. systems of coupled non-linear reaction laws. An additional complexity comes into play due to the lack of measurability of individual physical quantities. Then the

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model regression method becomes highly non-linear in the model parameters.

The work should consist of the following steps:

i) Preparation of a general plasma-chemical reaction set for basic catalytic processes relevant for CO2 dissociation (Langmuir-Hinshelwood, Eley-Rideal etc.)
ii) Literature research and implementation of surface reactions on different catalysts.
iii) In-depth numerical analysis of relevant scenarios to identify important reaction channels in the interaction of plasma chemistry and surface reactions.

The task for the Master's thesis consists of a combination and modification of existing FORTRAN sub-routines such that an extended flexibility for model identification is possible. This might be extended by a module for a quantitative estimate of the quality of model regression.

Date*	Signature*
14.04.2020	Dirk Reiser

* required field