2016 Jülich – OCPC – Programme
for the involvement of postdocs in bilateral collaboration projects

PART A

Title of the project: Development of an *ab initio* description of electronic transport across silicon oxide based passivation layers in silicon heterojunction solar cells

Jülich's institute: Institute of Energy and Climate Research 5 - Photovoltaics

Project leader: Dr. Urs Aeberhard

Web-address: http://www.fz-juelich.de/iek/iek-5/EN/Forschung/Abteilung%20AS/AG%20Theorie/AG_Theorie_node.html

Description of the project: see overleaf

Description of existing or sought Chinese collaboration partner institute:
The partner institute should have a strong research focus on computational materials science, preferably in the field of photovoltaics or energy materials.

Required qualification of the post-doc:

- PhD in physics, with theoretical/computational focus
- Experience with molecular dynamics and *ab initio* transport simulation (DFT + NEGF) as applied to semiconductor materials and devices
- Good knowledge of scientific english (spoken and written) and presentation skills

PART B

Documents to be provided by the post-doc:

- Detailed description of the interest in joining the project (motivation letter)
- Curriculum vitae, copies of degrees
- List of publications
- 2 letters of recommendation

PART C

Additional requirements to be fulfilled by the post-doc:

- Max. age of 33 years
- PhD degree not older than 5 years
- Very good command of the English language
- Strong ability to work independently and in a team

Description of the project:

The silicon heterojunction device is one of the main candidates for the next industrial standard for high-efficiency silicon solar cells. The core of the technology consists of the application of passivating contact layers to reduce minority carrier losses at the silicon wafer surface. Different silicon alloys have been proposed and implemented as passivation layers, such as a-Si:H, a-SiO_x or a-SiO_2.
While record-high solar cell efficiencies could be reached in practise, the fundamental mechanisms of charge carrier transport and recombination at the heterointerface are still not well understood. This is in part due to the amorphous nature of the passivation layers, featuring a plethora of electronic states with different degree of localization and distributed over a large energy range, but also to the large band offsets and strong doping-induced band bending in the heterojunction region, which invalidates the application of the semi-classical picture conventionally used in solar cell device modelling.
A proper description of transport and recombination of photogenerated charge carriers at the heterointerface should thus combine an atomistic description of the interface including the doping induced potential with a quantum-kinetic formalism of the charge carrier dynamics. In this way, the different transport channels from direct, defect- and phonon assisted tunneling to thermionic emission can be treated on equal footing and consistently with the interband recombination.
The target material system will be the newly introduced a-SiO_2 TOPCon (Tunnel Oxide Passivated Contact). As the first step in the project, the atomic structure of the a-SiO_2 – c-Si interface will be constructed by *ab initio* molecular dynamics simulations. The electronic and vibrational information obtained from DFT will then be used to parametrize a mesoscopic Hamiltonian for the quantum kinetic transport formalism. Transport across the interface will be computed on both ballistic and inelastic levels, using the Büttiker-Landauer approach and the full Meir-Wingreen formalism including the electron-phonon interaction self-energy.
The computational resources required for the project will be provided by the Jülich Supercomputing Centre, which hosts one of the largest supercomputing infrastructures in Europe. The project will be carried out in close collaboration with the experimental activities of the Silicon Heterojunction Materials and Solar Cells group headed by Dr. Kaining Ding.