SOPHIA European Research Infrastructure	**Modelling and Simulation**	**Forschungszentrum Jülich GmbH** **Name of the platform: JUROPA**
Location of the infrastructure :	**Wilhelm-Johnen-Strasse, Jülich, Germany**	http://www.fz-juelich.de/ias/jsc/juropa/
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Objectives :	• Large-scale, computation-intensive material and device simulations for photovoltaic applications
Main features :	• General purpose parallel SMP-cluster JUROPA • 2,208 compute nodes with 2 quad-core Nehalem-EP processors each • 207 Tflops peak performance • File server and disk storage capabilities • Access to pre-installed software packages on JUROPA for various applications in quantum chemistry, physics, engineering and visualisation • Technical support from the Jülich Supercomputing Centre staff for porting, benchmarking and optimization of application codes on the specific supercomputing architecture in close collaboration with the applicant • Access to experimental material data for the calibration of models, provided by the IEK5-Photovolaics at Forschungszentrum Jülich
Limitations or constraints :	Compute power of 25,000 Tflop-hours will be provided subject to the regulations of TNA and upon a thorough review process considering both scientific quality of the proposal and the compliance with the technical requirements, which are • Minimum number of cores per job: 8 (1 node) • Maximum RAM per node (8 cores): 22 GB • Maximum 512 nodes • Proof of scaling under production conditions with I/O
Typical services or results :	Efficient calculation of computationally demanding simulations on a high-end supercomputing infrastructure
Examples of research projects :	• Optical simulations of realistic solar cell structures (including rough interfaces, nanoparticles, plasmonic effects, etc) via rigorous solutions of Maxwell's equations in 3D • Optoelectronic simulation of novel solar cell devices with nanostructured absorbers (quantum wells, -wires and –dots) • Modelling of material growth in thin-film solar cell devices • Ab-initio investigation of defect formation in solar cell devices, e.g. at interfaces, under illumination, etc.