

Dr. Piotr Kowalski

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Jülich Young Investigator Group: Atomistic Modeling for Nuclear Technology



„My goal is to establish a virtual laboratory that utilizes modern computational methods and resources for atomistic modeling of materials relevant for nuclear technology, in particular for the nuclear waste management.“

Research project:

The group uses advanced quantum chemistry software and superior computational resources available at FZJ for atomistic simulations of materials important for nuclear waste management. Our simulations reveal crucial information about the atomic-scale mechanisms governing

the interaction of radionuclides with various materials, including these considered as future nuclear waste forms. Our main goal is to complement the ongoing experimental research on radionuclide-bearing materials by providing information on electronic structure, thermodynamical

stability, spectral signatures and radiation damage processes. The long-term goal of such a joint theoretical and experimental studies aims at the development and characterization of new, advanced materials for safe management of nuclear waste.

What is/has been the greatest challenge as head of a young investigators group:

Efficient and mutually beneficial management of skills and talents of group members and obviously acquiring third party funding.

Start of funding period: July 2012
End of funding period: June 2017
Budget: € 250 000/year
Staff: 2 PhD students and 1 Postdoc

University affiliation: foreseen RWTH Aachen

Cooperations: University of Frankfurt, Benemerita Universidad Autonoma de Puebla (Mexico) Curtin Univesity (Australia), University College London