

## ***ThUL School on Actinide Chemistry 2017***

**Forschungszentrum Jülich GmbH  
Jülich, Germany**

*16-20 October 2017*

We kindly invite young researchers to attend the ThUL school on computational actinide chemistry that will be organized this year by the Institute of Nuclear Waste Management (IEK-6) at Forschungszentrum Jülich GmbH (FZJ – Research Centre Jülich). The school will cover the main topics related to atomistic modeling of actinide-bearing materials with the lecturing focusing on the combination of computational modeling and experimental techniques for characterization of nuclear waste materials. Besides the strictly topic oriented lectures and practical exercises, the attendants will have an opportunity to learn about the modern, large computational resources hosted by the research center, development of computational software, research performed at the Research Centre Jülich and in the Institute of Nuclear Waste Management in principle.

The school follows a decade long tradition of similar meetings. Previous schools were held in Lille (2006), Cadarache (2007), Karlsruhe (2012-15) and Dresden (2016). Following these successful schools, the 2017 school will be held at the Forschungszentrum Jülich from 16 to 20.10.2017.

Forschungszentrum Jülich GmbH with more than 5000 employees is one of the largest research centers in Europe. It conducts research in the fields of Materials Science, Energy, Climate and Supercomputing. It hosts some of the most powerful computational resources and historically is renowned for nuclear science-related research, with the current focus on nuclear waste management.

The school is aimed at early career scientists (PhD students and postdocs) in the area of computational and experimental chemistry, physics and materials science of actinide-bearing materials. **The language of the school is English and the attendance is free of charges.**

The school will consist of lectures and practical sessions in computational actinide science. The topics will be of general character and are aimed at a more general audience

### **Contributors to the ThUL School**

A number of experts in the field of computational and experimental actinide science will give lectures on theoretical, numerical and experimental aspects of this and related research fields. The contributors to the school will be:

Evgeny Alekseev (FZJ, Germany)  
Dirk Bosbach (FZJ, Germany)  
Christoph Friedrich (FZJ/PGI-1, Germany)  
Nina Huittinen (HZDR Dresden, Germany)  
Sandro Jahn (U. of Köln, Germany)  
Piotr Kowalski (FZJ, Germany)  
Kristina Kvashnina (ESRF, France)  
Nigel Marks (Curtin U., Australia)  
Michael Patzschke (HZDR Dresden, Germany)  
Jenna Poonoosamy (FZJ, Germany)  
Robert Polly (KIT, Germany)  
Bernd Schimmelpfennig (KIT, Germany)  
Victor Vinograd (FZJ, Germany)  
Daniel Wortmann (FZJ/PGI-1, Germany)

### **Nuclear Waste Management**

Nuclear waste has been accumulating world wide as a side effect of nuclear energy production and other nuclear and non-nuclear (e.g. mining) industrial activities. There is a world-wide consensus on the deep geological disposal of the waste and currently a scientific basis for the safe disposal is being formulated. This requires investigation of materials properties and processes that influence and determine the long-term behavior of the waste and incorporation of actinide elements into different materials phases. In recent years computational methods of quantum chemistry and

materials science become very popular research tools that are frequently utilized for the research on the nuclear waste materials.

### Computational Actinide Sciences

With the steady, exponential increase in the availability of supercomputing power and advancement in the computational software, especially in the *ab initio*-based codes, at the beginning of XXI century the field of computational materials science emerged as an important and growing research activity. *Ab initio* calculations of materials have become an integral part of many scientific papers and a very popular research technique in the field of nuclear materials, including nuclear waste.

*f*-elements such as actinides are not only experimentally, but also computationally very challenging. Various effects related to the strongly-correlated character of *f* electrons and strong spin-orbit interaction must be understood and properly taken into account in order to make computations reliable and predictable. Various aspects of these computations will be discussed during the school and covered by practical computer exercises that will illustrate challenges faced by computational actinide science.

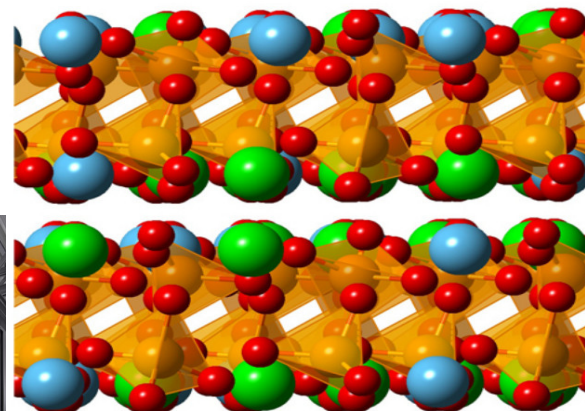
### 2017 ThUL school

By organizing the ThUL school at Forschungszentrum Jülich we provide the attendees a unique opportunity to interact with the experts on computational and experimental aspects of actinide science, get knowledge on the related modern supercomputing activities and learn interdisciplinary approaches to the research. The attendees will also have the opportunity to get familiar with the research ongoing at the research center, visit labs related to nuclear waste management research and get a first-hand overview on the general supercomputing activities.

**Persons interested in attending the ThUL school should contact Dr. Piotr Kowalski**  
([p.kowalski@fz-juelich.de](mailto:p.kowalski@fz-juelich.de))

We are looking forward to welcome you to Jülich for a very educative and enjoyable week with actinides and supercomputers.

On behalf of the organizers  
Piotr Kowalski



Organizing committee:

Piotr Kowalski (Head, FZJ, Jülich, Germany)  
Michael Patzschke (HZDR, Dresden, Germany)  
Robert Polly (KIT, Karlsruhe, Germany)

