



ThUL Questionnaire

Dear colleague,

The Theoretical Userlab (ThUL) is a component of the European sixth framework Network-of-Excellence ACTINET (<http://www.actinet-network.org/>) which aims to foster the development of theoretical methods suitable for the investigation of actinide chemistry and physics, and to stimulate discussion and joint projects between theory and experiment in this field. So far, the main work of the ThUL has been to organise combined theoretical/experimental schools and workshops (http://www.actinet-network.org/theoretical_user_lab). We are also seeking to establish the key issues that both experimentalists and theoreticians believe can be aided by contributions from the other, as well as to identify the computer resources (both hardware and software) required by the theoreticians in order to allow them to address these issues, with a view to providing the resources within ACTINET.

In order to help us in our work, we would like to ask you to kindly answer the questions raised below:

- Are there computational methods you consider to be highly beneficial in this context, which are currently not available due to lack of financial support for their development and implementation? To which type of questions could such software be applied?
- Would you be interested in using dedicated hardware and preinstalled software for tackling challenging questions in actinide science, if they were provided by the ThUL/ACTINET (on the basis of peer-reviewed proposals)? Which type of hardware would be most suitable in your opinion, and what is the minimum resource (CPU-weeks, disk space and memory) you would require in order to make it worthwhile for you to write a proposal?
- What do you see as being the principal current technical obstacles to computational actinide science?
- Which experiments on actinide compounds do you consider to be most crucial as reference data for benchmarking or calibrating theoretical approaches?
- Which topics should in your opinion be covered at the joint theory/experiment schools and workshops which the ThUL organises?

Space intentionally left blank for your comments:

Your answers, comments, questions and suggestions are highly welcome on this flyer, in electronic form or during a personal discussion at a conference.

Sincerely

The ThUL Task Group

Bernd Schimmelpfennig (Chair, Bernd.Schimmelpfennig@ine.fzk.de)

Valérie Vallet (valerie.vallet@univ-lille1.fr)

Nik Kaltsoyannis (n.kaltsoyannis@ucl.ac.uk)

François Jollet (francois.jollet@cea.fr)

Address (snail mail):

Bernd Schimmelpfennig

Forschungszentrum Karlsruhe GmbH

Institut für Nukleare Entsorgung(INE)

P.O.B. 3640

D-76021 Karlsruhe

Germany