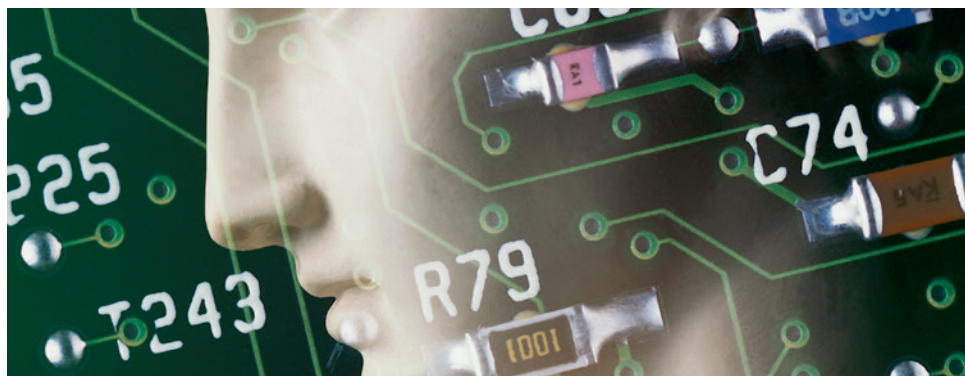


# Computational chemistry and materials' modelling services



## Industry Scope

The Multiscale Materials Modelling group offers computational chemistry and materials' modelling services to a broad range of industries:

- Chemicals
- Pharma
- Battery
- Nuclear

## PSI provides the following services

Consultancy and Research projects varying from purely applied industry R&D based towards academic, requiring more of fundamental research:

- Customer tailored, flexible duration agreements
- Short term consulting services, starting from one person month
- Longer academia industry projects in the framework of postdoctoral or PhD studentships
- Confidential, non-publishable projects

## Methodology and scope of activity

We apply state of the art computational tools in the framework of the Density Functional Theory, Semi Empirical and Force Field potentials, using static and Molecular Dynamics calculations. Our research portfolio includes a spacious spectrum of molecules, materials and process simulations studies. These include and are not limited to:

Chemical  
Reactivity

Solid State  
Chemistry

Energy Viable  
Materials

Characterization

Workflow  
construction

Critical literature  
review

PSI welcomes your  
proposals

- **Chemical Reactivity:** Reaction mechanisms, Homogeneous and heterogeneous catalysis
- **Solid State Chemistry:** Band gap and band structure, Mechanical response of materials, Polymorph stability, Ionic diffusion in structured solids
- **Energy Viable Materials:** Reduction and oxidation potentials, electrode voltages, Electrocatalysis
- **Characterization:** IR, Raman, Optical absorption spectroscopy, X-ray absorption spectroscopy
- **Workflow construction** using python, bash scripting
- **Critical literature review**
- **PSI welcomes your proposals** for joint cooperation in a broad area of atomistic computer simulations

## Contact

### Paul Scherrer Institut

Dr. Matthias Krack  
OHSA/D07  
Forschungsstrasse 111  
5232 Villigen PSI  
Switzerland

Tel. +41 56 310 58 56  
matthias.krack@psi.ch  
[www.psi.ch/de/lsm/mmm-group](http://www.psi.ch/de/lsm/mmm-group)

