

Workshop Program

The Joint DMG and BMBF-IMMORAD Verbundproekt
Workshop "*From atomistic calculations to thermodynamic
modelling*" (18-22 February 2013, Frankfurt a. M.)

Note: The Workshop will be preceded by the IMMORAD Meeting, which will occupy the whole day of Monday 18.02

Monday 18.02

9.00-9.45 *Arrival*

9.45-10.30 ***ImmoRad Meeting presentations***

10.30-11.00 *Coffee break*

11.00-11.45 ***ImmoRad Meeting presentations***

11.45-13.15 *Lunch*

13.15-14.00 ***ImmoRad Meeting presentations***

14.00-14.45 ***ImmoRad Meeting presentations***

14.45-15.15 *Coffee break*

15.15-18.00 ***ImmoRad Meeting presentations***

18.00-19.00 ***ImmoRad posters/Workshop registration***

Tuesday 19.02

9.00-9.45 **D. Bosbach.** Nuclear Waste Management: Challenges

9.45-10.30 **M. Prieto.** *Solid solution-aqueous solution systems*

10.30-11.00 *Coffee break*

11.00-11.45 **M.T. Dove.** *Introduction to Structure Modelling*

11.45-13.15 *Lunch*

13.15-14.00 **M.T. Dove.** *Introduction to Quantum Chemistry*

14.00-14.45 **V. Milman.** *Introduction to Density Functional Theory*

14.45-15.15 *Coffee break*

15.15-18.00 ***Materials Studio/Tutorial***

19.00-22.00 ***Dinner***

Wednesday 20.02

9.00-9.45 **A.V. Plyasunov.** *Thermodynamics of Aqueous Species*

9.45-10.30 **J.D. Gale.** *Simulation of Solid/Aqueous Interfaces*

10.30-11.00 *Coffee break*

11.00-11.45 **J.D. Gale.** *Simulation of Solid/Aqueous Interfaces*

11.45-13.15 *Lunch*

13.15-14.00 **F. Heberling.** *Thermodynamics of Se(IV) Incorporation in Carbonates*

14.00-14.45 **T. Stumpf.** *Actinides in Carbonates: Spectroscopic Methods*

14.45-15.15 *Coffee break*

15.15-18.00 ***Aqueous Species Tutorial/ Materials Studio Tutorial***

18.00-20.00 ***Workshop posters***

Thursday 21.02

9.00-9.45 **P. Kowalski.** *Actinide Compounds from DFT*
9.45-10.30 **V.L. Vinograd.** *Virtual Solid Solution Laboratory*
10.30-11.00 *Coffee break*
11.00-11.45 **A. Belonoshko.** *Thermodynamics from Molecular Dynamics*
11.45-13.15 *Lunch*
13.15-14.00 **A. Belonoshko.** *Thermodynamics from Molecular Dynamics*
14.00-14.45 **F. Brandt/M. Klinkenberg** *Incorporation of Ra in Barite*
14.45-15.15 *Coffee break*
15.15-18.00 **Materials Studio Tutorial**
18.00-19.00 **Excursion to the labs (High-Pressure, PPMS and Crystal Physics)**

Friday 22.02

9.00-9.45 **D. Kulik.** *Gibbs Energy Minimization*
9.45-10.30 **GEMS-3 Tutorial**
10.30-11.00 *Coffee break*
11.00-11.45 **GEMS-3 Tutorial**
11.45-13.15 *Lunch*
13.15-14.00 **GEMS-3 Tutorial**
14.00-14.45 **Individual projects**
14.45-15.15 *Coffee break*
15.15-18.00 **Individual projects/Departure**