Universität für Bodenkultur Wien
University of Natural Resources and Applied Life Sciences, Vienna

Department of Materials Sciences and Process Engineering
Institute of Chemical and Energy Engineering
Professor Dr.-Ing. Martin Wendland, Professor Dr. Johann Fischer

POSTDOC POSITION AVAILABLE

Molecular Modelling and Simulation in Chemical Engineering: Adsorption from aqueous solutions

The Priority Research Program 'Molecular Modelling and Simulation in Chemical Engineering' with international participation is financed by Deutsche Forschungsgemeinschaft. In this program, the project 'Adsorption from aqueous solutions' was granted to our Institute of Chemical and Energy Engineering in Vienna, Austria.

Adsorption from liquid solutions and in particular from aqueous solutions is of great practical interest. Molecular modelling of this process, however, is less developed than for adsorption from the gas phase. An additional challenge is adsorption from dilute or demixing solutions. So far, we have modelled adsorption via the Potential of Mean Force (PMF), which is determined by integration of the mean force calculated with MD simulations [1-3]. Future work shall concentrate on the improvement of the method by non-equilibrium MD simulations or density functional theory [4]. Finally, the results shall be used for developing engineering models.

The position is open for a postdoc for a period of two years and is paid according to Austrian FWF conditions (http://www.fwf.ac.at/de/projects/personalkostensaetze_2008.html).

Please send applications with CV and list of publications until February, 17th 2008 to Professor M. Wendland by mail (Institut für Verfahrens- und Energietechnik, Universität für Bodenkultur, 1190 Muthgasse 107, Wien, Austria) or e-mail. Reprints of the referenced and related papers of our Institute can be requested for further information by e-mail.

BOKU seeks to increase the percentage of female employees and strongly encourages qualified women to apply. Applicants are not entitled to reimbursement of travel and subsistence expenses incurred by the selection and interviewing procedure.

[1] W. Billes et al., Langmuir **19,** 10862-10868 (2003).

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[2] W. Billes et al., Molecular Simulation **33**, 655-666 (2007).

[3] R.Tscheliessnig et al., Adsorption from oversaturated aqueous solution: Mean force molecular simulations, submitted for publication.

[4] K. Bucior et al., J. Chem. Phys. **126,** 094704, 1-10 (2007)

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