

# DFG Priority Program 1362

## February 24-25

Technical University Dresden, Hörsaalzentrum  
Bergstraße 64, 01069 Dresden

<b>Topical Workshop – MOF Modelling for PhD students</b>
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### February 24, 2009, presentations:

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| 09.00-09.10 | Introduction: Prof. Dr. Stefan Kaskel (University of Dresden)  |
| 09.10-09.55 | Dr. Tina Düren (University of Edinburgh)<br>“Force field calculations of MOFs: Introduction and Examples”                |
| 09.55-10.40 | Dr. Frank Hoffmann (University of Hamburg)<br>“Molecular Modelling of MOFs: Introduction to computer exercises”          |
| 10.40-11.10 | Coffee break   |
| 11.10-11.55 | Dr. Rochus Schmid (University of Bochum)<br>„Accurate First Principles Derived Force Fields for Porous Hybrid Materials” |
| 11.55-12.55 | Lunch Break  |
| 12.55-15.30 | Computer exercises/ Examples: Force field calculation  |
| 15.30-16.00 | Coffee break   |
| 16.00-18.00 | Computer exercises/ Examples: Force field calculation  |

## February 25, 2009, presentations:

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| 09.00-09.45 | Prof. Dr. Gotthard Seifert (University of Dresden)<br>“DFT based calculations on the structure and properties of MOFs”                              |
| 09.45-10.15 | Dr. Igor Baburin (Max- Planck-Institute Dresden)<br>“Topology analyses of MOFs”   |
| 10.15-10.45 | Coffee break  |
| 10.45-11.15 | Dr. Sergei Yurchenko (University of Dresden)<br>“Theoretical approaches to the simulation of the hydrogen adsorption in nano- porous substrates”    |
| 11.15-12.00 | Dr. Agnieszka Kuc (Jacobs University Bremen)<br>“DFTB calculations on the structures and properties of MOFs:<br>Introduction to computer exercises” |
| 12.00-13.00 | Lunch break   |
| 13.00-15.30 | Computer Exercises/ Examples: DFT calculation   |
| 15.30-16.00 | Coffee break  |
| 16.00-18.00 | Computer Exercises/ Examples: DFT calculation   |