

Summer School 2009 Computational Chemistry and Spectroscopy September 22 – 25, 2009 Hotel Bredeney, Essen



Program

Tuesday, September 22, 2009

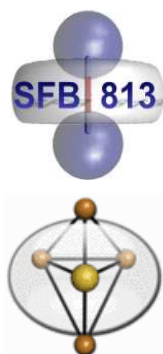
- 18.00 *Dinner*
20.00 Keynote Lecture
Prof. Dr. Wolfgang Lubitz, Mülheim an der Ruhr: „Magnetic Resonance Studies on Metalloenzymes: Hydrogenase and the Oxygen Evolving Complex“

Wednesday, September 23, 2009

- 09.00 Prof. Dr. Frank Neese: „Introduction to Quantum Chemical Methods“
10.15 *Coffee Break*
10.45 Dr. Frank Wennmohs: „Fundamentals of Computational Chemistry“
12.00 *Lunch*
14.00 Prof. Dr. Frank Neese: „Introduction to the ORCA Program System“
16.00 *Coffee Break*
16.30 Practical Courses
17.00 Special Interest Groups
1. Relativistic Effects in Open-Shell Spectroscopy (Dr. Dmitri Ganiouchine)
2. Molecular Dynamics (Dr. Frank Wennmohs)
18.00 *Dinner*
20.00 Postersession I

Thursday, September 24, 2009

- 09.00 Prof. Dr. Frank Neese: „Ligand Field Theory“
10.15 *Coffee Break*
10.45 Prof. Dr. Frank Neese: „Quantum Chemistry of Open-Shell Molecules“
12.00 *Lunch*
14.00 Practical Courses
16.00 *Coffee Break*
16.30 Practical Courses
17.00 Special Interest Groups
1. Electron Correlation Methods: Theory and Application (Andreas Hansen)
2. QM/MM Methods for Large Molecular Systems (Christoph Riplinger)
18.00 *Dinner*
20.00 Postersession II



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Friday, September, 25, 2009

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| 09.00 | Prof. Dr. Frank Neese: „Optical Spectroscopy of Open-Shell Molecules“ |
| 10.15 | <i>Coffee Break</i> |
| 10.45 | Prof. Dr. Frank Neese: „EPR Spectroscopy and Quantum Chemistry“ |
| 12.00 | <i>Lunch</i> |
| 14.00 | Practical Courses |
| 16.00 | <i>Coffee Break</i> |
| 16.30 | Practical Courses |
| 17.00 | Special Interest Group The Theory of Effective Hamiltonians (Prof. Dr. Frank Neese) |
| 18.00 | <i>Dinner</i> |