



Seminar "Junior Research Group - Theoretical Bioinorganic Chemistry"

Date: 01. 12. 2010
Location: Department of Chemistry, Humboldt-Universität zu Berlin
Brook-Taylor-Str. 2, 12489 Berlin

Program

- 13.30 Lectures
Lecture Hall Building, Marie-Curie-Lecture Hall 0'06
- 13.30 **Claudio Greco, PhD** (Departement of Biotechnology and Biosciences, University of Milan-Bicocca)
Theoretical studies of [FeFe]-hydrogenases: from DFT modeling of bioinspired diiron models up to QM/MM treatment of the whole enzyme
- 14.15 **Dr. Petra Imhof** (Interdisciplinary Center for Scientific Computing, Ruprecht-Karls-University of Heidelberg)
Towards Biomimetic Catalysts
- 15.00 **Francesco Aquilante, PhD** (Department of Physical Chemistry, Geneva University)
The "spin problem" in transition-metal compounds and possible routes to its solution

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