



Vortragsankündigung

- im Rahmen des UniCat-Kolloquiums -
(www.unicat.tu-berlin.de)

Es spricht: **Prof. Dr. Per Siegbahn**
Department of Physics, Quantum Chemistry
Group, Stockholm University

Zeit: **Mittwoch, 26.11.2008**
17:15 Uhr

Ort: **TU Berlin**
Institut für Chemie, Altes Chemiegebäude
Straße des 17. Juni 115
10623 Berlin
Raum C230

Thema: **"Quantum chemistry and biological catalysis:
Towards mechanistic models of water
oxidation and heterolytic hydrogen cleavage"**

Abstract: Hybrid density functional theory has been used to study the mechanisms of a large number of transition metal containing enzymes. Over the years the models have become larger and more realistic. The present strategy for treating these systems will be described. DFT studies on the mechanism for dioxygen formation in photosystem II is then described. After the first X-ray structures of PSII appeared a few years ago, the understanding of this fundamental reaction has improved significantly. For example, during the past year major progress has been made concerning quantum chemically determined structures of the S-state intermediates. A detailed mechanistic proposal will be presented including a complete energy diagram. At the end of the talk, a new mechanism will also be presented for heterolytic hydrogen cleavage by NiFe-hydrogenase.

Organisator: Prof. Dr. Dau (FUB)

Gäste sind herzlich willkommen!

Prof. Dr. Matthias Drieß
Sprecher des Exzellenz-Clusters UniCat