

## Fachartikel

### PSII

- P. Liebisch, C. Müller, M. Grabolle, M. Haumann und H. Dau (2005). Simulation of XANES spectra for protein-bound metal centers: Analysis of linear dichroism data. *Physica Scripta*: in Druck.
- P. Liebisch und H. Dau (2005). The linear dichroism in the X-ray absorption near-edge spectra of imperfectly, unidirectionally oriented samples - Theoretical approach and application to the protein-bound manganese complex of photosystem II". Manuskript in Vorbereitung.
- P. Liebisch, und H. Dau (2005). The catalytic cycle of photosystem II studied by simulation of X-ray absorption near edge spectra - Manganese oxidation versus ligand radical formation. Manuskript in Vorbereitung.
- M. Haumann, P. Liebisch, C. Müller, M. Barra und H. Dau (2005). Intermediate formation in photosynthetic water oxidation followed by a time-resolved X-ray absorption experiment. Manuskript in Vorbereitung.
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- A. Magnuson, P. Liebisch, M. Haumann, J. Höglom, M. F. Anderlund, R. Lomoth, W. Meyer-Klaucke und H. Dau (2005). Bridging-mode changes in response to manganese oxidation in two binuclear manganese complexes - implications for photosynthetic water-oxidation. *Journal of Biological Inorganic Chemistry*: eingereicht.

- M. Haumann, P. Pospisil, M. Grabolle, C. Müller, P. Liebisch, V. A. Sole, T. Neissius, J. Dittmer, L. Iuzzolino und H. Dau (2002). First steps towards time-resolved BioXAS at room temperature: State transitions of the manganese complex of oxygenic photosynthesis. *Journal of Synchrotron Radiation* 9: 304-308.
- Müller, C., P. Liebisch, M. Barra, H. Dau und M. Haumann (2004). The location of calcium in the manganese complex of oxygenic photosynthesis studied by X-ray absorption spectroscopy at the Ca K-edge. *Physica Scripta*: in Druck.

### Hydrogenasen

- M. Haumann, A. Porthun, T. Buhrke, P. Liebisch, W. Meyer-Klaucke, B. Friedrich and H. Dau (2003). Hydrogen-induced structural changes at the nickel site of the regulatory NiFe hydrogenase from *Ralstonia eutropha* detected by X-ray absorption spectroscopy. *Biochemistry* 42(37): 11004-11015.
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### Hämocyanin

- P. Liebisch, H. Hartmann, C. Müller, D. Hönig, K.-H. Decker und H. Dau (2005). The influence of pH on the oxygen-binding binuclear copper site of hemoxyanin in *Eurytelma californicum* and *Palinurus elephas*. Manuscript in Vorbereitung.

### Biogene Manganablagerungen

- A. Schöler, P. Liebisch, C. Müller, C. Plieth. und H. Dau (2005). Volcano-shaped manganese deposits at the cell wall of green alga *Chara corallina* - Elemental mapping and comparative structural analysis by spatially resolved X-ray microfocus experiments. Manuscript in Vorbereitung.

### Vanadium-haltige Bromoperoxidase

- U. Christmann, H. Dau, M. Haumann, E. Kiss, P. Liebisch, D. Rehder, G. Santoni and C. Schulzke (2004). Substrate binding to vanadate-dependent bromoperoxidase from *Ascophyllum nodosum*: A vanadium K-edge XAS approach. *Dalton Transactions*(16): 2534-2540.

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- M. Haumann, A. Porthun, T. Bührke, P. Liebisch, T. Burgdorf, W. Meyer-Klaucke, B. Friedrich und H. Dau (2002/2003). The Ni-Fe centers of oxygen-insensitive hydrogenases from *Ralstonia eutropha* studied by Ni-XAS. HASYLAB/EMBL - Annual Report.
- A. Magnuson, P. Liebisch, M. Haumann, S. Styring, W. Meyer-Klaucke und H. Dau (2002). Comparison of structural changes at the native manganese complex of photosystem II with manganese model compounds by means of XAS. HASYLAB/EMBL - Annual Report.
- M. Haumann, A. Porthun, P. Liebisch, C. Müller, T. Burgdorf, W. Meyer-Klaucke, B. Friedrich und H. Dau (2001). Hydrogen-sensing Ni-Fe site of regulatory hydrogenase. HASYLAB/EMBL - Annual Report.
- H. Dau, M. Haumann, M. Barra, P. Liebisch und C. Müller (2003). The manganese complex of photosynthetic water oxidation in all S-states at 10 K - Polarization dependent XAS, ESRF - Annual Report
- H. Dau, M. Haumann, M. Barra, P. Liebisch und C. Müller (2003). Structural changes of the tetra-manganese complex of oxygenic photosynthesis during the oxygen-evolving transition induced by Laser-flashes and studied by timeresolved BioXAS, ESRF - Annual Report.
- H. Dau, M. Haumann, M. Barra, P. Liebisch und C. Müller (2003). The calcium binding site at the manganese complex of oxygenic photosynthesis: Investigations by calcium XAS on native and biochemically treated photosystem II, ESRF - Annual Report.
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- H. Dau, M. Haumann, M. Grabolle, P. Liebisch und C. Müller (2002). The manganese complex of photosynthetic water oxidation studied by calcium EXAFS, ESRF - Annual Reports.

## Ausgewählte Konferenzbeiträge

- P. Liebisch und H. Dau. Simulation of XANES spectra for protein-bound metal centers: Analysis of linear dichroism data. XAFS12, 22. - 27. Juni 2003, Malmö, Schweden, (Vortrag)
- P. Liebisch, M. Grabolle, M. Haumann, C. Müller und H. Dau. XANES of protein-bound metal centers: Oxidation state changes of the photosynthetic manganese complex and other systems. European Conference on Bioinorganic Chemistry (EUROBIC), 30. Juli - 6. August 2002, Lund, Schweden, (Poster)
- P. Liebisch, , C. Müller, M. Haumann und H. Dau. X-ray Absorption Spectroscopy on Metallo-Enzymes (BioXAS); BESSY user workshop, 14. April 2002, Berlin, (Vortrag)
- P. Liebisch, M. Grabolle, M. Haumann, C. Müller und H. Dau. XANES-Simulationen für protein-gebundene Metallzentren: Der PSII-Mangankomplex und andere Systeme. 8. - 11. September 2002, Jahrestagung der Deutschen Gesellschaft für Biophysik, Dresden, (Poster)