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## COMPUTATIONAL SCIENCE COLLOQUIUM

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organized by the Computational Science Initiative at the JKU

### Invitation

to a public talk (with following discussion)

- Title: **„Theory of optical spectra of photosynthetic pigment-protein complexes: From structure to function”**
- Lecturer: Univ.-Prof. Dr. Thomas Renger  
(Institute for Theoretical Physics, University of Linz)
- Date: Wednesday, **Dez 16, 2009, 17:15**
- Place: **HF 9901**, University of Linz

In photosynthesis the light energy absorbed by so-called antenna pigment-protein complexes is transferred to the photosynthetic reaction center where it is converted into chemical energy. An important open question is: How does the protein trigger excitation energy transfer? The latter can occur with nearly hundred percent quantum efficiency.

To address this question, a dynamical theory of optical spectra is combined with a structure-based electrostatic/quantum chemical computation of the parameters of the theory. The methods are applied to photosynthetic pigment-protein complexes of green sulfur bacteria and cyanobacteria. Quantitative agreement of the calculated optical spectra with the experimental data is obtained allowing to analyse the structure-function relationships in detail.