# PHYSIKALISCHES KOLLOQUIUM

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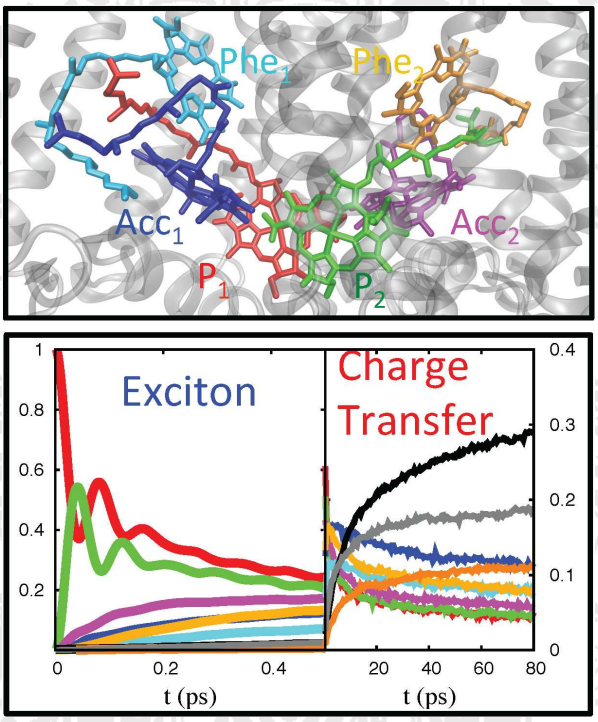
IM GROßEN HÖRSAAL




## QUANTUM AND SEMICLASSICAL DYNAMICS OF COMPLEX MOLECULES

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We outline a partial linearized density matrix (PLDM) propagation scheme to explore excitation energy transfer and charge separation dynamics in extended dissipative models of biological light harvesting systems. The approach is formulated in terms of models of the many electron wave functions. Our studies include excited state energy transfer inside light harvesting domains, between these domains and the reaction center (RC), and finally the dynamics of conversion of excitation energy to charge separation inside the RC complex. Parts of our model pathways involve strongly coupled pairs, or dimers of chromophores that often act as intersections between transmission paths composed largely of monomers. These dimers give rise to quantum beats and we explore their influence on the partitioning of amplitude flow between different intersecting pathways for realistic parameterization of the pigment-protein environment coupling as well as the influence of static site disorder in our model. New results are also presented exploring excitation energy transfer pathways in the other light harvesting systems where dissipation to high frequency quantal vibrational modes plays a key role in determining the dominant pathway for energy transfer through this extended complex. Time permitting, we will also outline a new approach for using our PLDM propagation scheme with a one electron orbital representation that requires semiclassical treatment of fermion anti commutation. This promising new area of research that I plan to explore during my visit to FRIAS, has the potential to include many electron correlation explicitly in the dynamics.