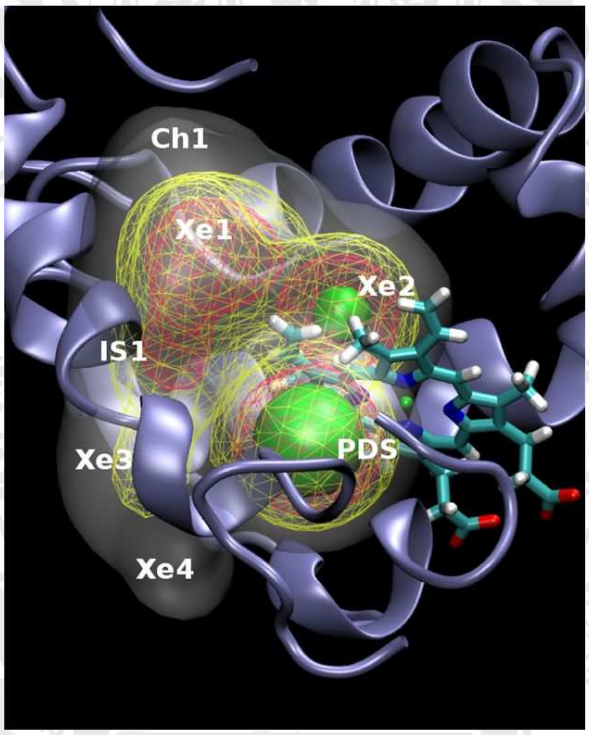
PHYSIKALISCHES KOLLOQUIUM

AM 26. NOVEMBER 2012 UM 17 UHR C.T.

IM GROßEN HÖRSAAL



PHYSICAL CHARACTERIZATION OF PROTEIN INTERIORS WITH SMALL DIATOMIC PROBES

PROF. DR. MARKUS MEUWLY

DEPARTMENT OF CHEMISTRY

UNIVERSITY OF BASEL, SCHWEIZ

Atomistic Simulations have provided deeper insights into biophysical processes on various time and length scales. An essential ingredient for this are accurate and physically meaningful intermolecular potential energy surfaces. After a brief introduction into modern approaches to describe intermolecular interactions and applications to controlled experiments I will focus on unravelling diffusion pathways, chemical reactivity and the coupling between ligand- and protein motion. Together with insights from 1D- and 2D-spectroscopies, a combined computational/experimental approach may provide biological insight into the function and dynamics of small protein engines.