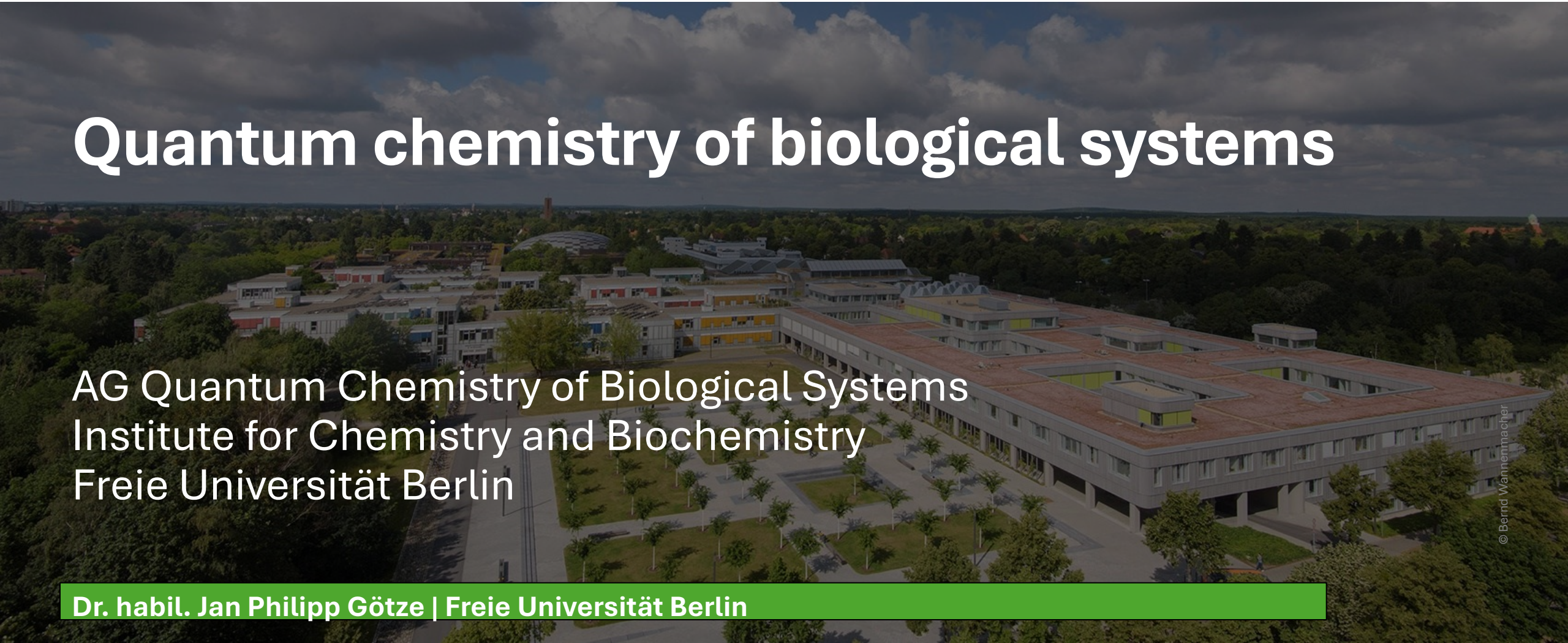
FREIE UNIVERSITÄT BERLIN

QC BioSys

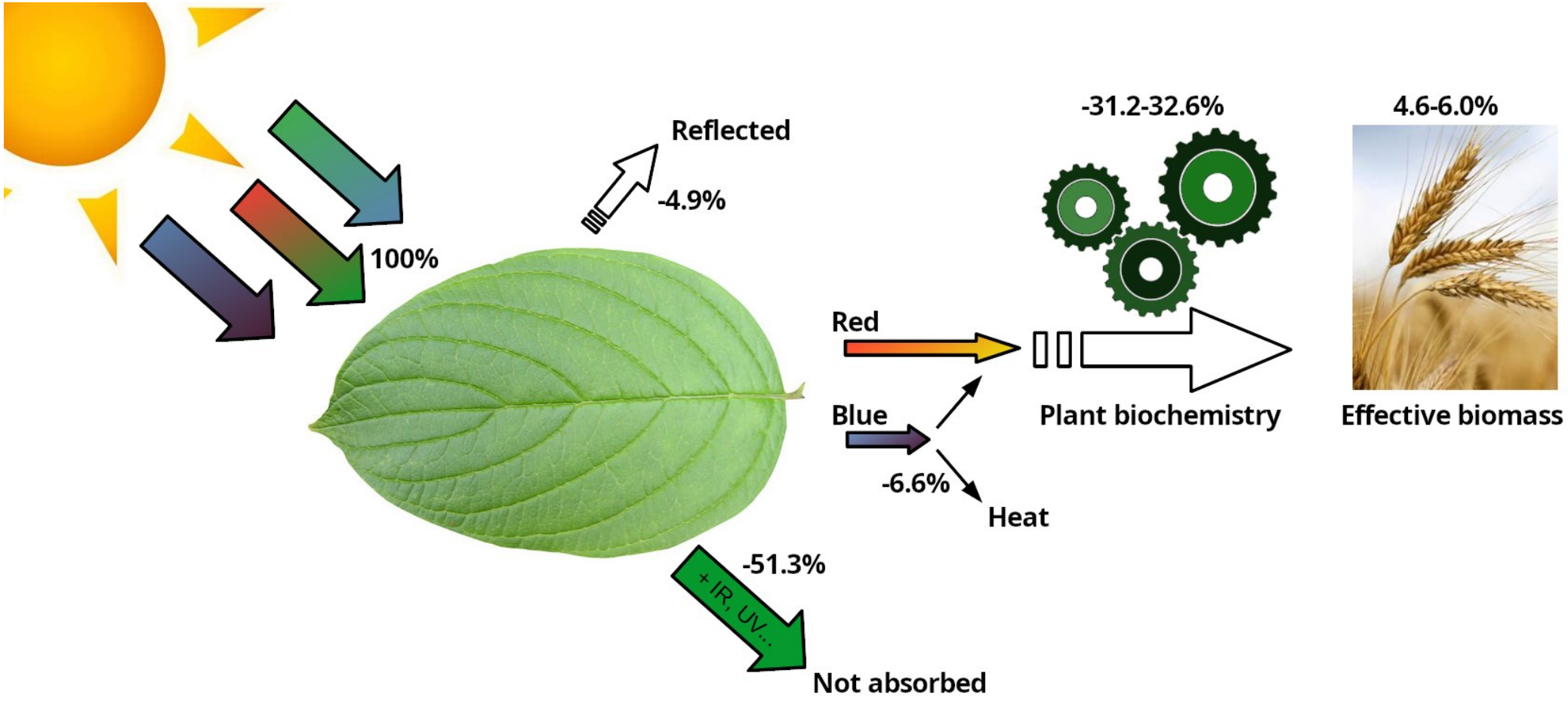
Quantum chemistry of biological systems



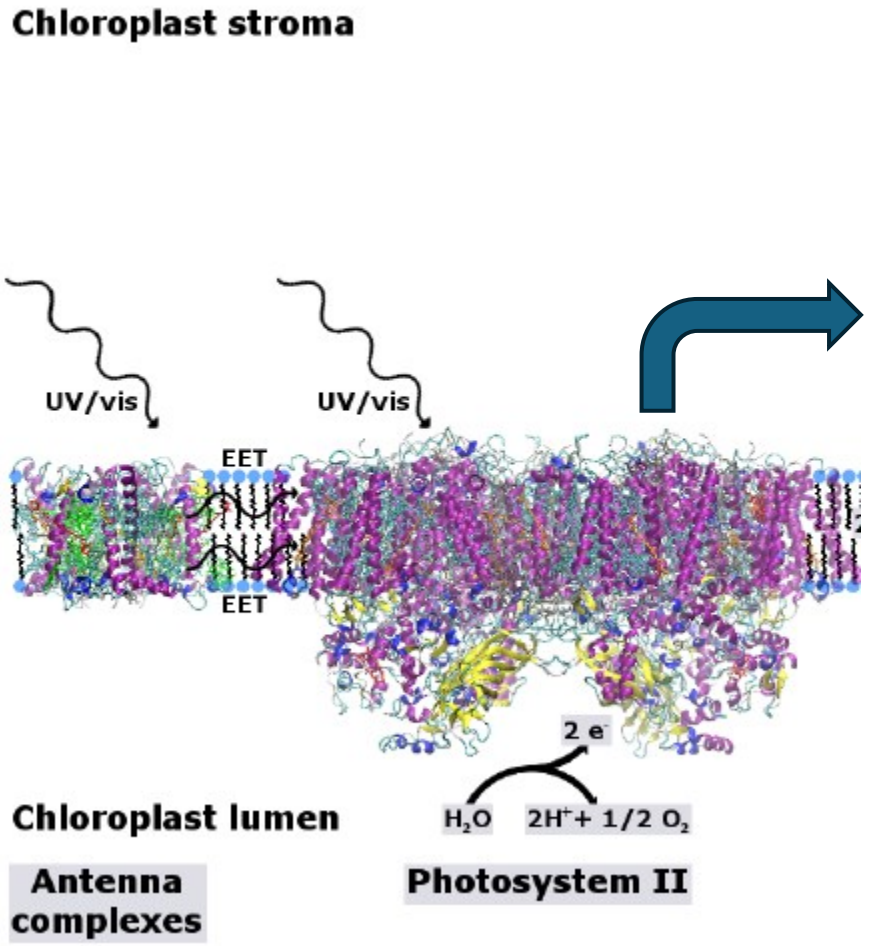
AG Quantum Chemistry of Biological Systems
Institute for Chemistry and Biochemistry
Freie Universität Berlin

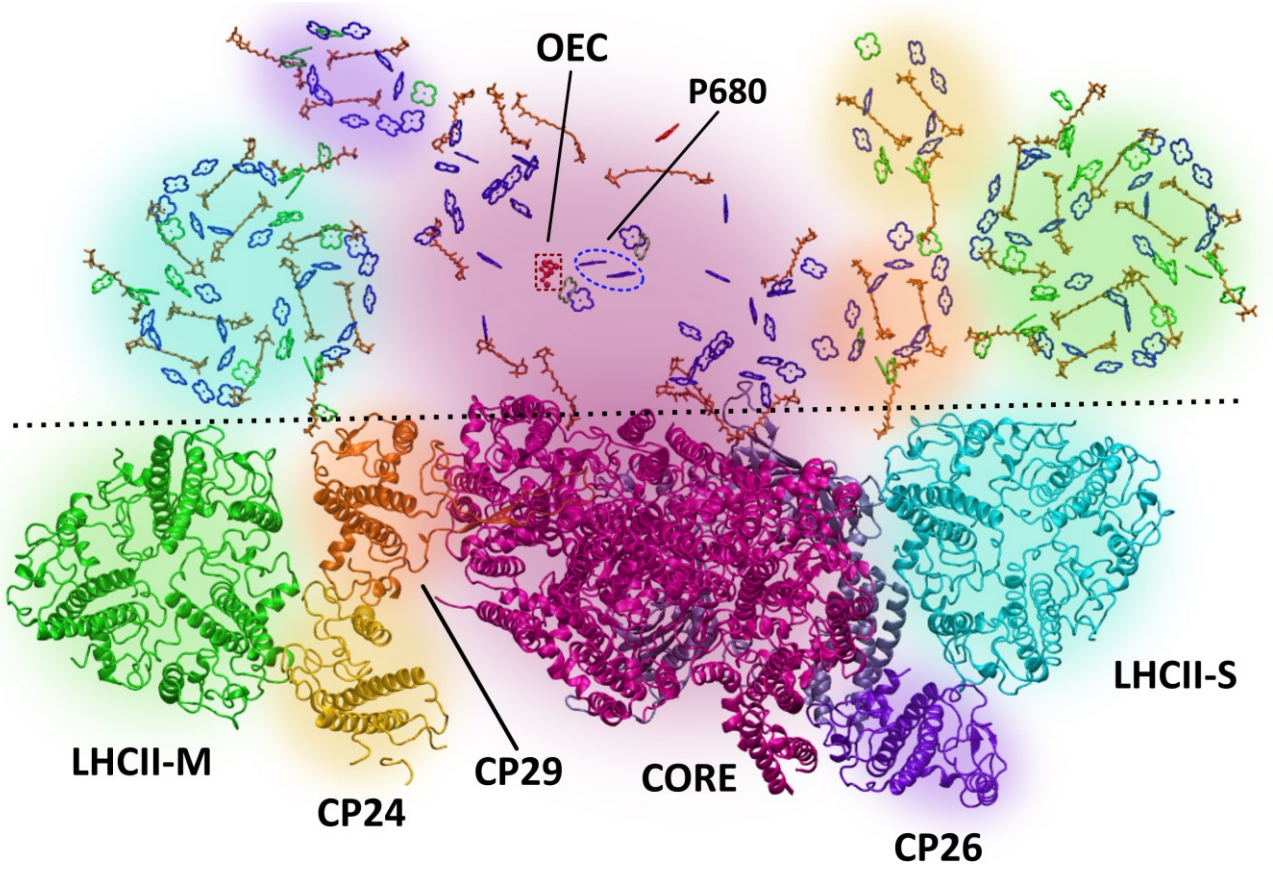
Dr. habil. Jan Philipp Götze | Freie Universität Berlin

Structure-function relationship in light harvesting



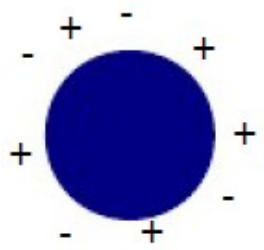
Structure-function relationship in light harvesting



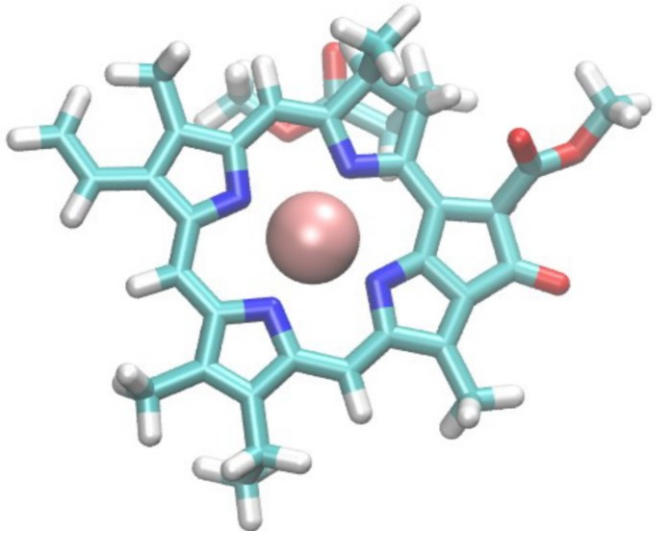


- Structure-function relationship not trivial
- Is every pigment needed? (Robustness)

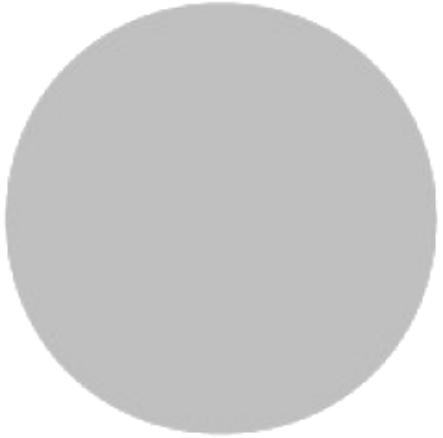
Theory approach

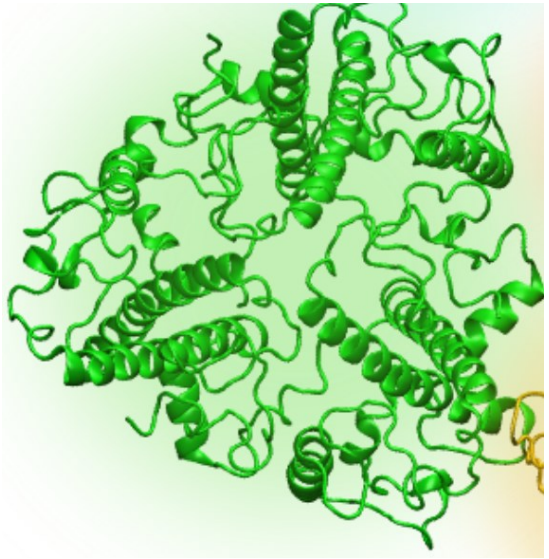


$$E_{QM,\,PCF}$$

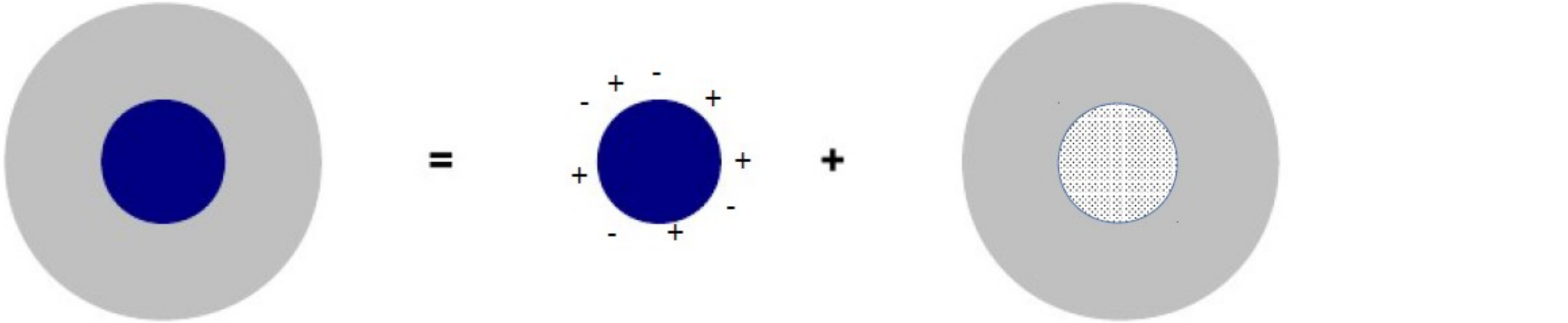


Theory approach



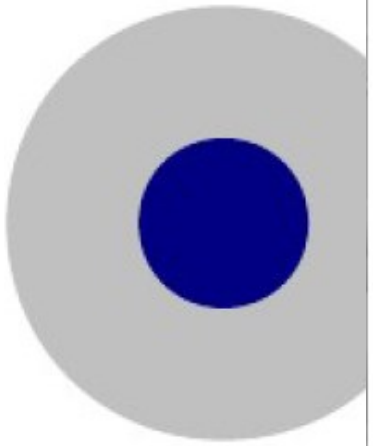


Theory approach

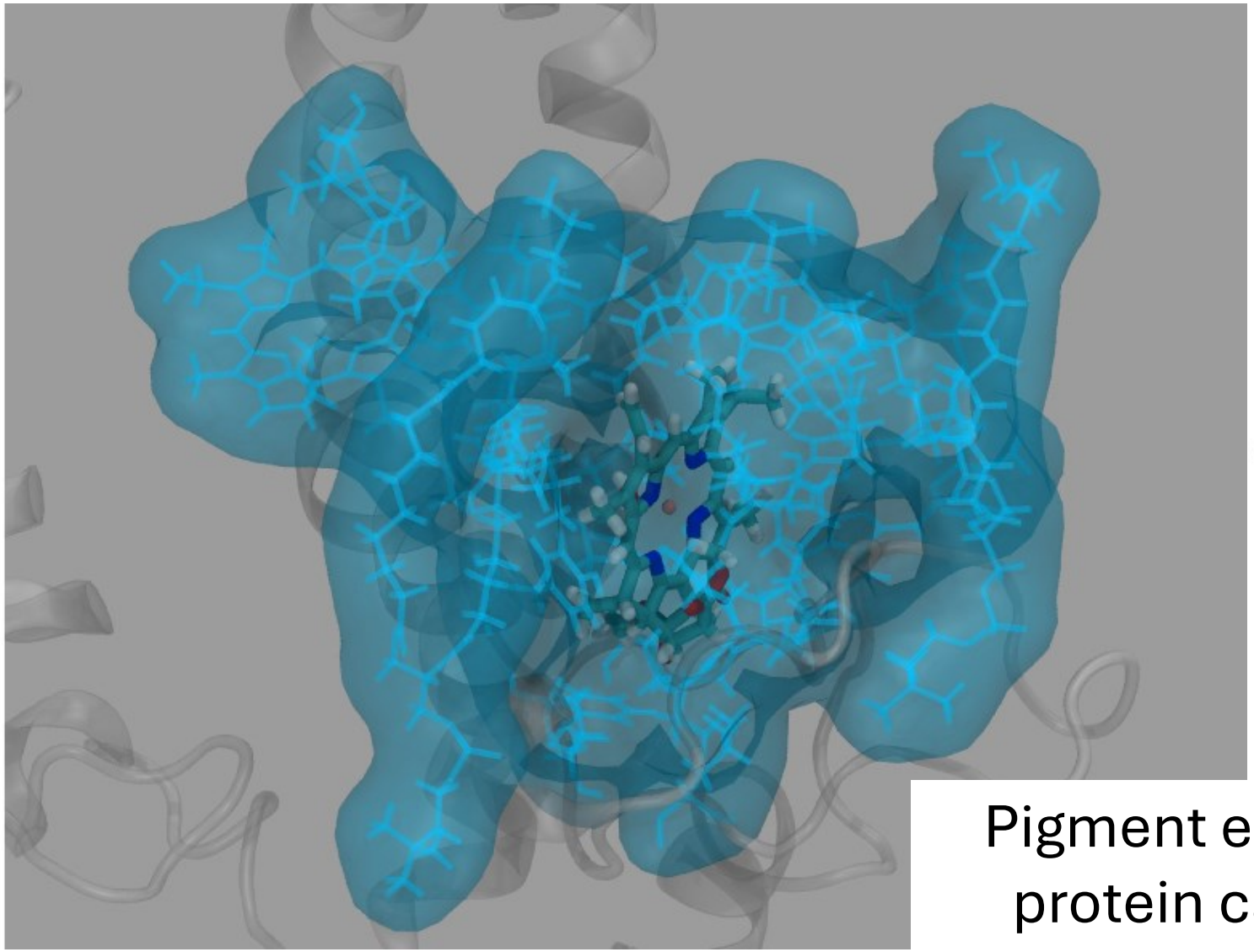


$E_{Add.\ QM/MM} = E_{QM,\ PCF} + E_{MM,vdW} \quad (+ \quad E_{Con})$

Theory approach



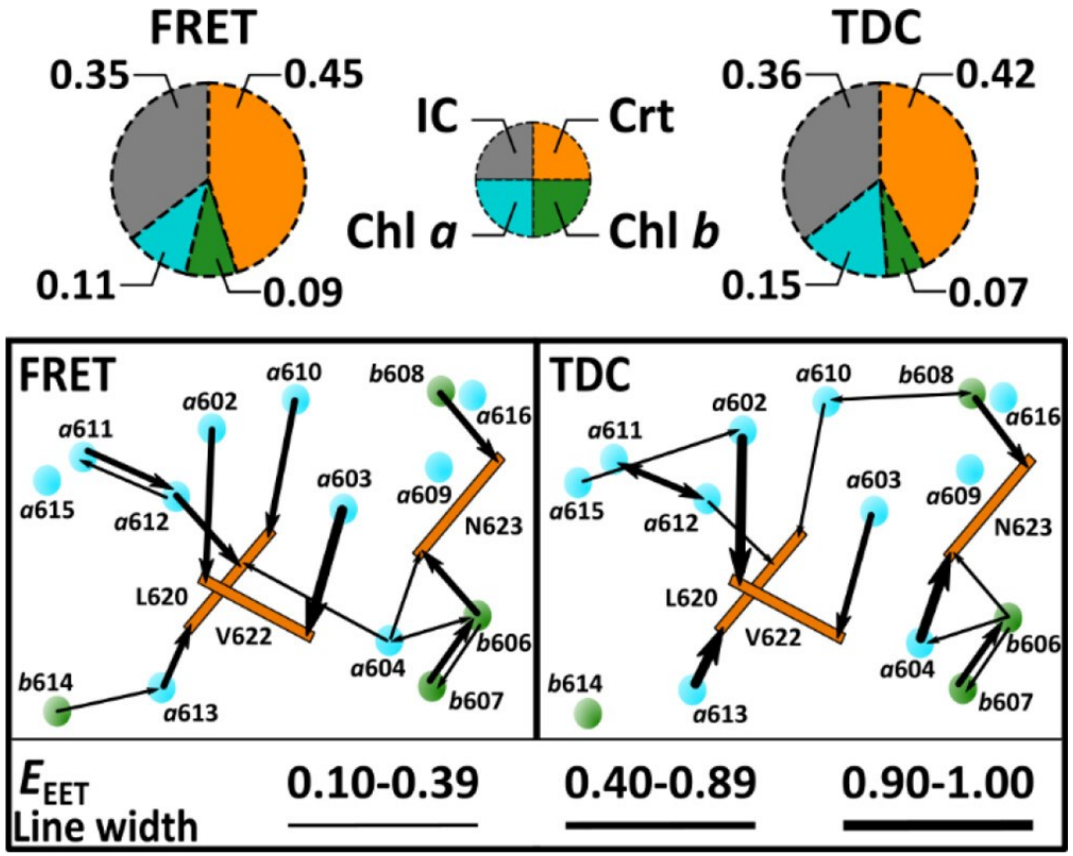
$E_{Add.\ QM/MM}$

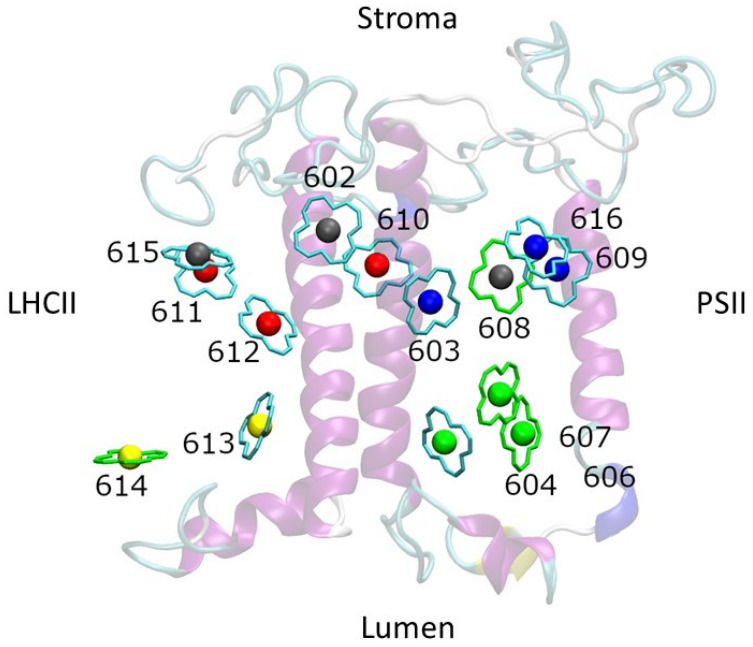


$(+ \quad E_{Con})$

Pigment embedded in a protein cage: QM/MM

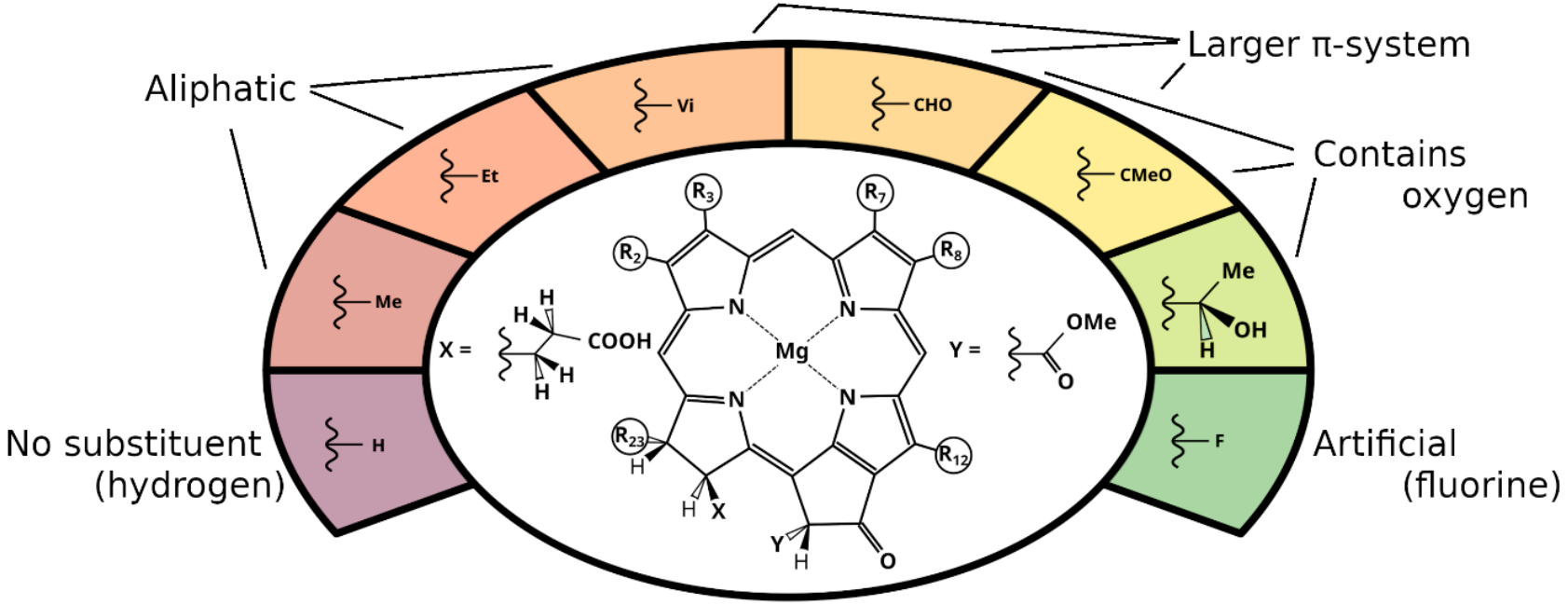
Calculating the energy networks of photosynthesis



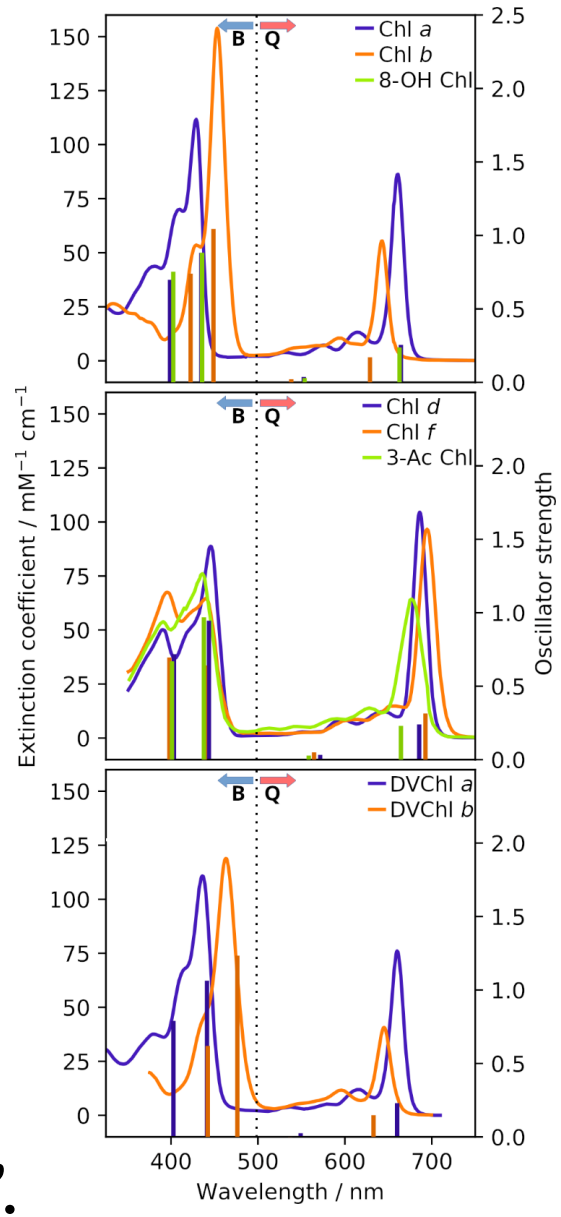


CP29 antenna protein

Prediction of new pigments: New chlorophylls



Set of 250.000 chlorophyll variants tested via machine learning



Exp. vs. ML

New chlorophylls available as synthetic “treasure maps”.

Weber et al. (2025) Photosynth Res, accepted

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Freie Universität Berlin

DFG Deutsche Forschungsgemeinschaft