

Neutron Scattering Experiments under Illumination and with Time-Resolution

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Outline

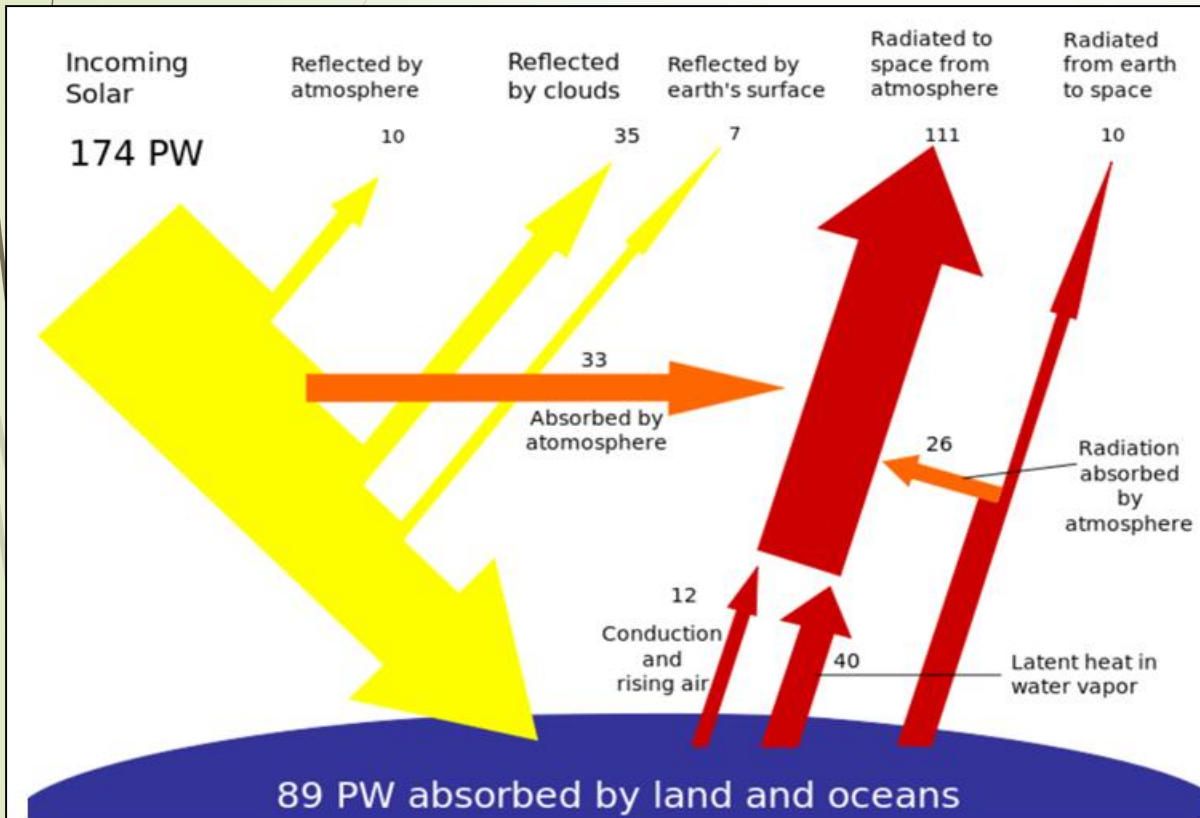
- Motivation
- Measurement under constant illumination
- Time-resolved measurement
- Concept of pump-probe cell
- Conclusions



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- **Motivation**
- Measurement under constant illumination
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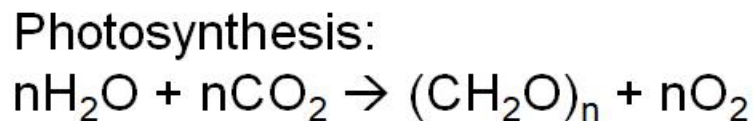
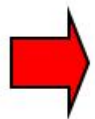
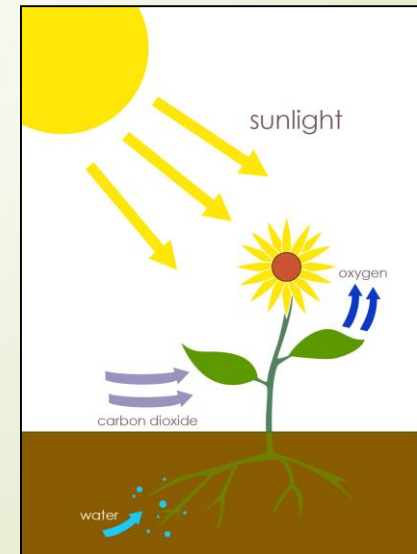
Motivation



Photosynthesis:

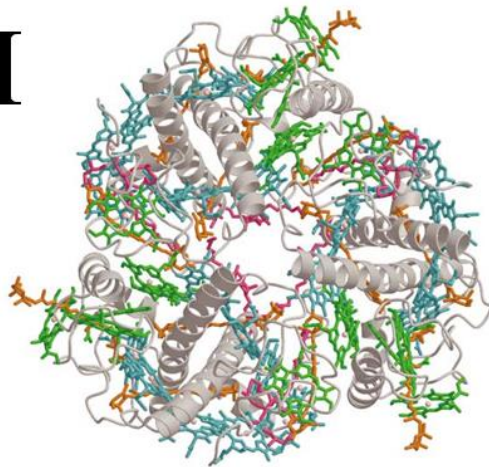
Transformation of light energy into storable chemical energy

Sufficient energy source in future



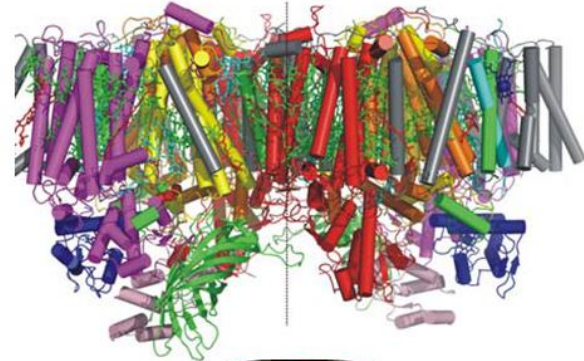
Motivation

I



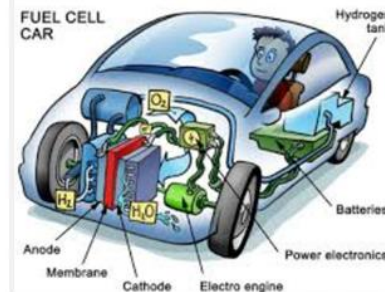
Light-harvesting
in antenna complex LHCII

II



Water splitting into hydrogen and
oxygen
in Photosystem II

more efficient
solar cells



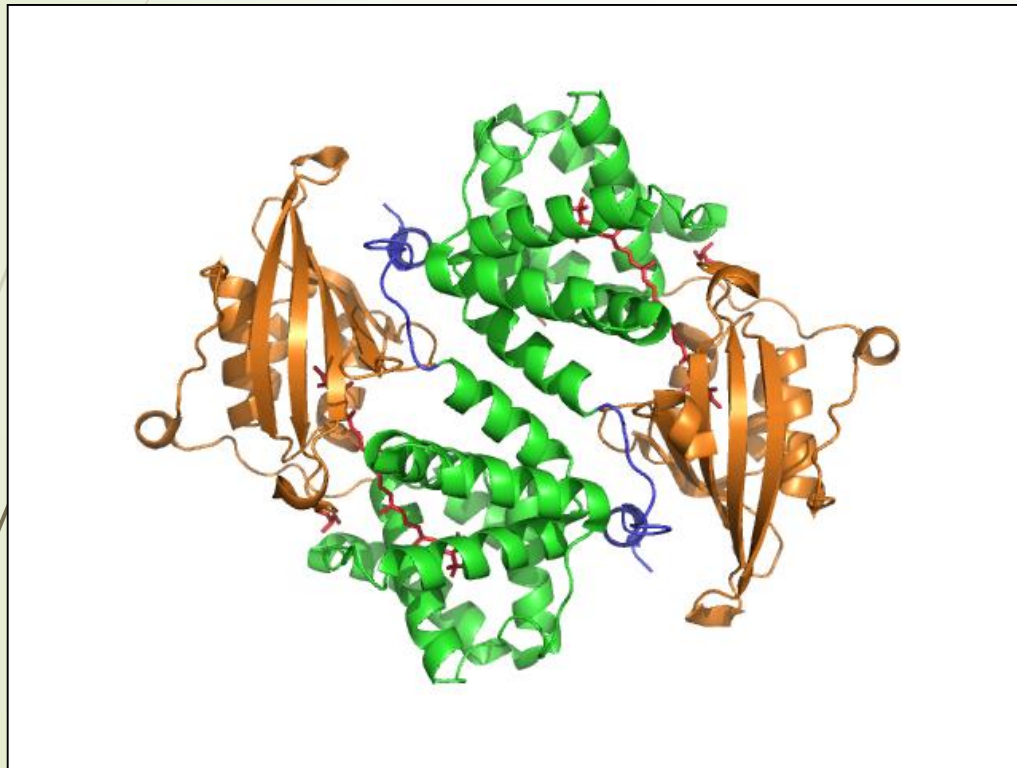
clean fuel



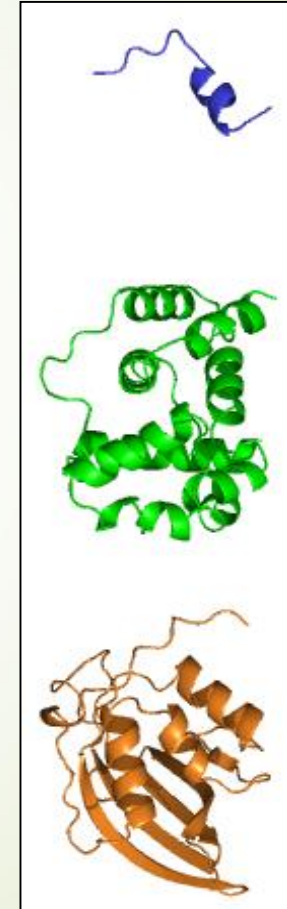
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Orange Carotenoid Protein



OCPwt dimer (pdb 3MG1)

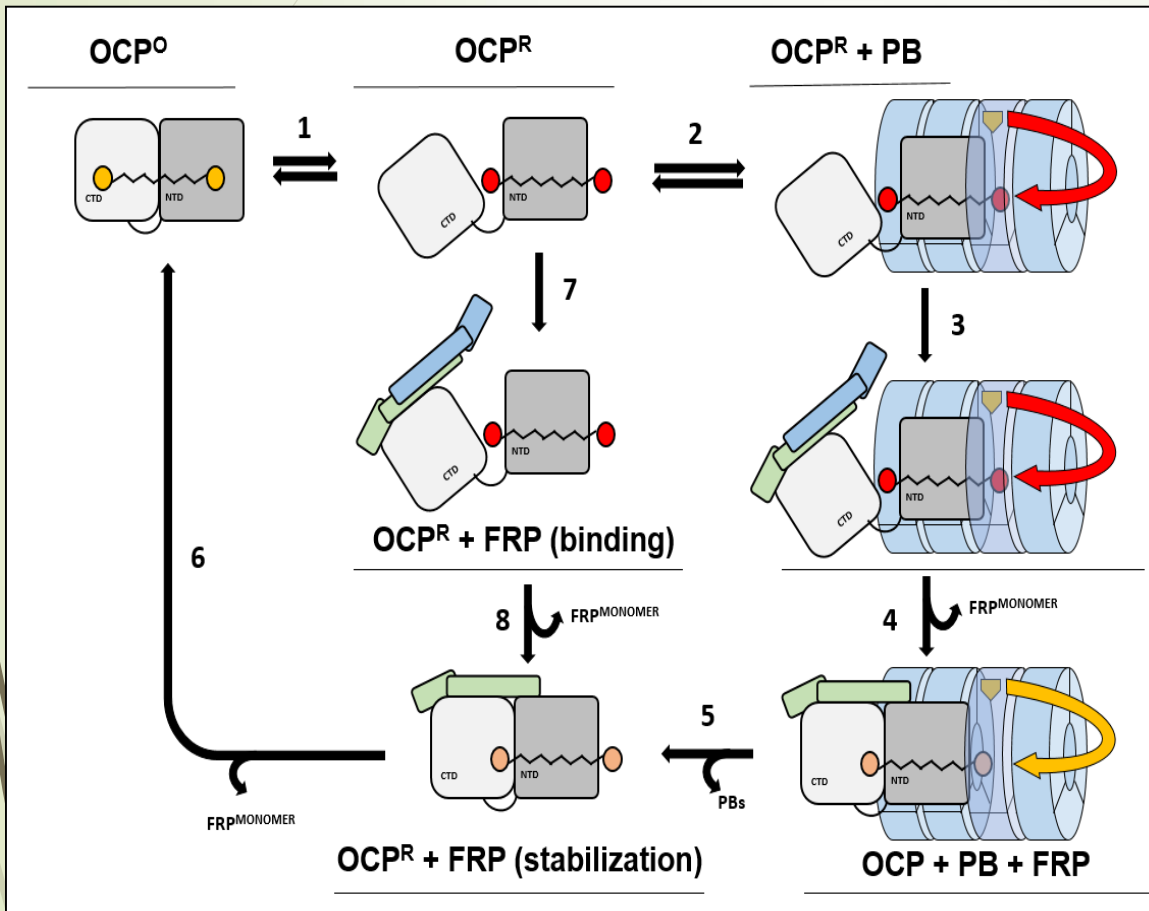


N-terminal

N-domain

C-domain

Orange Carotenoid Protein

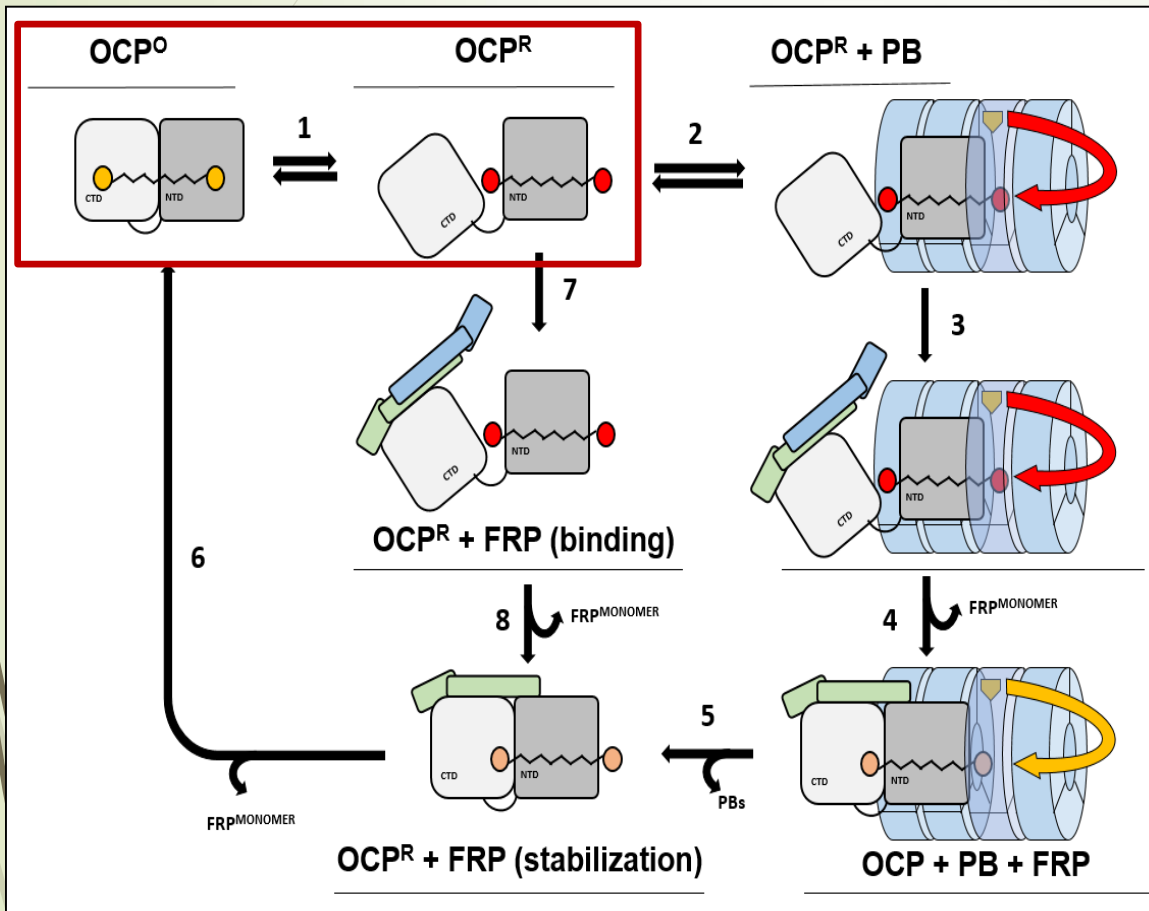


Functional role:

OCPwt is responsible for the non-photochemical quenching of phycobilisomes under intense blue light

Photo damage is prevented

Orange Carotenoid Protein

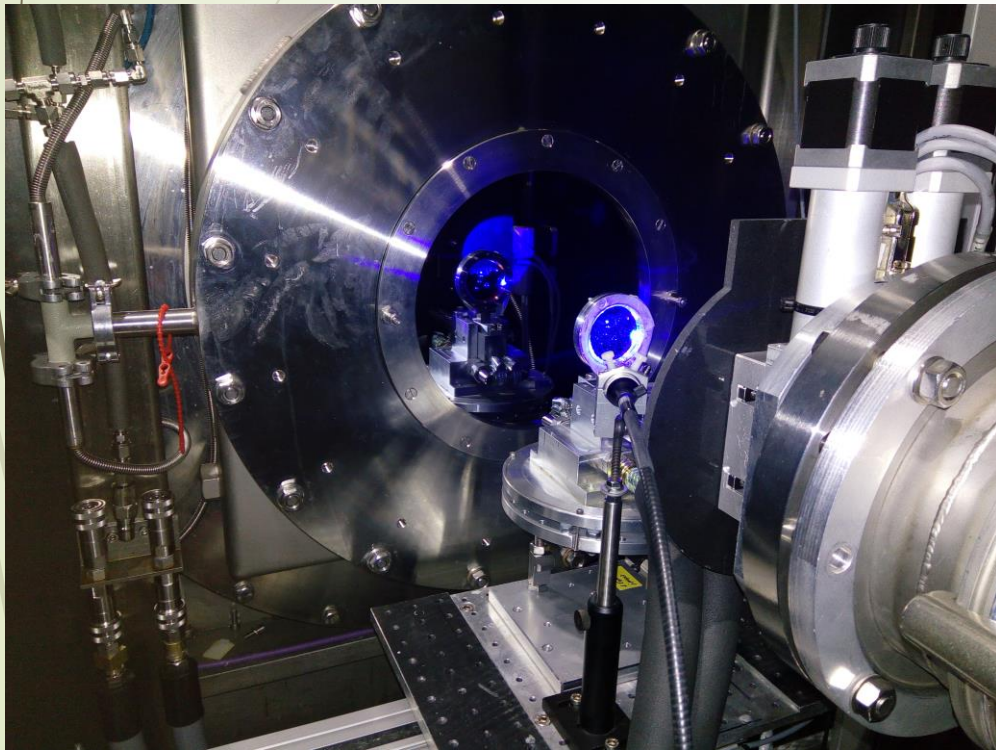


Functional role:

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Structural Pre-characterization



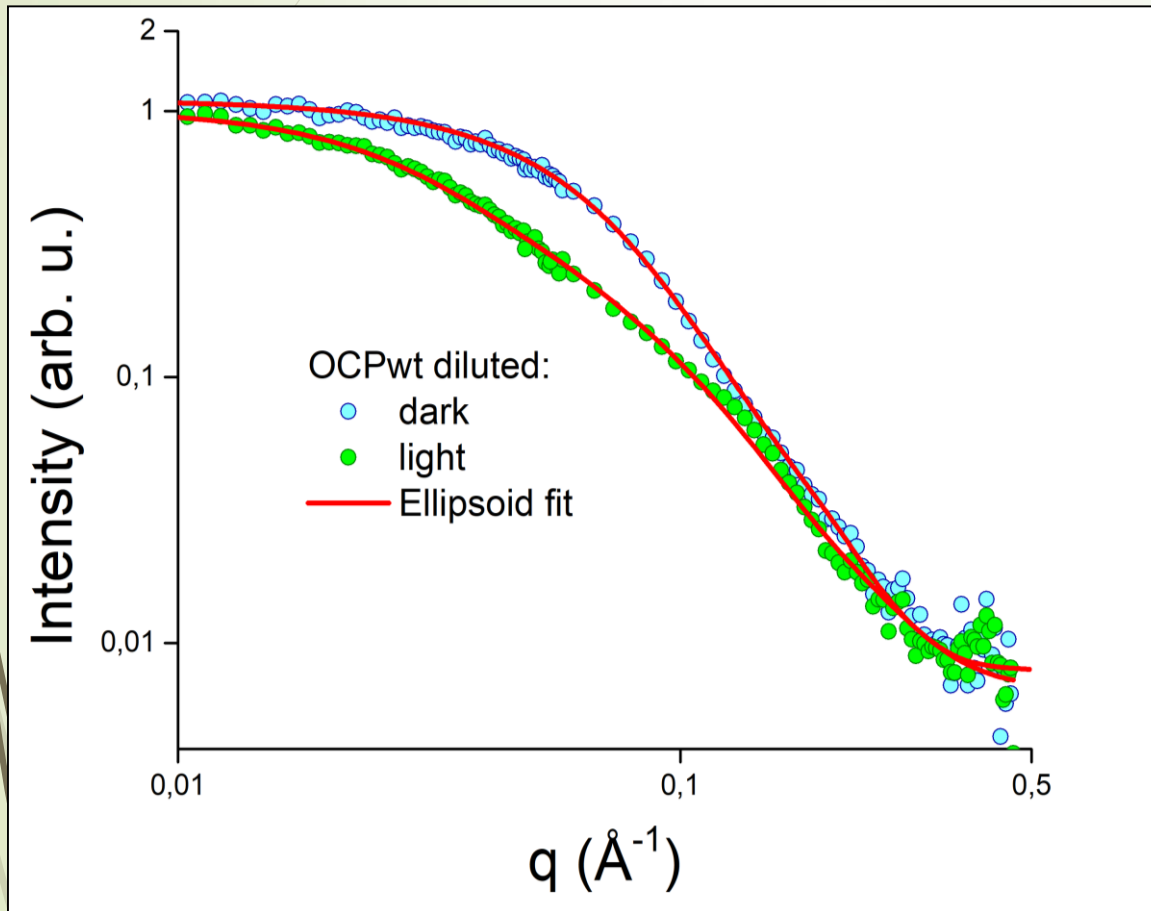
Instrument platform



Sample cell

KWS 1 (FRMII)

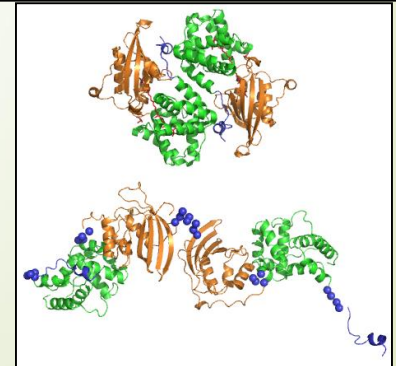
SANS Light Effect



SANS results:

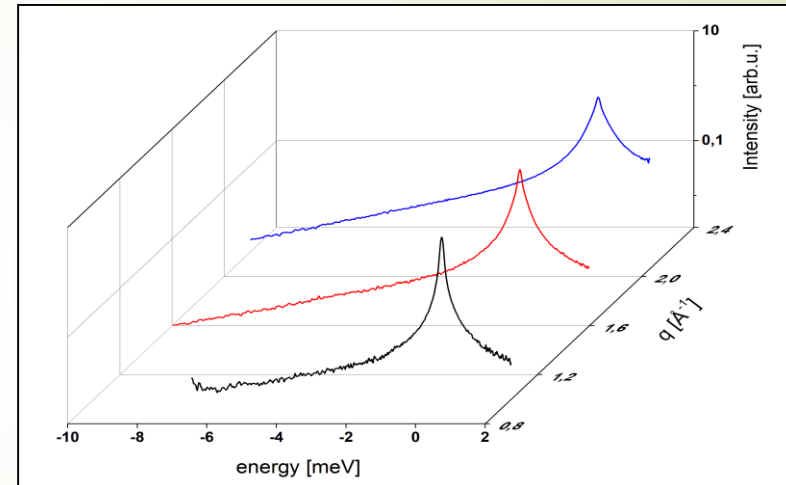
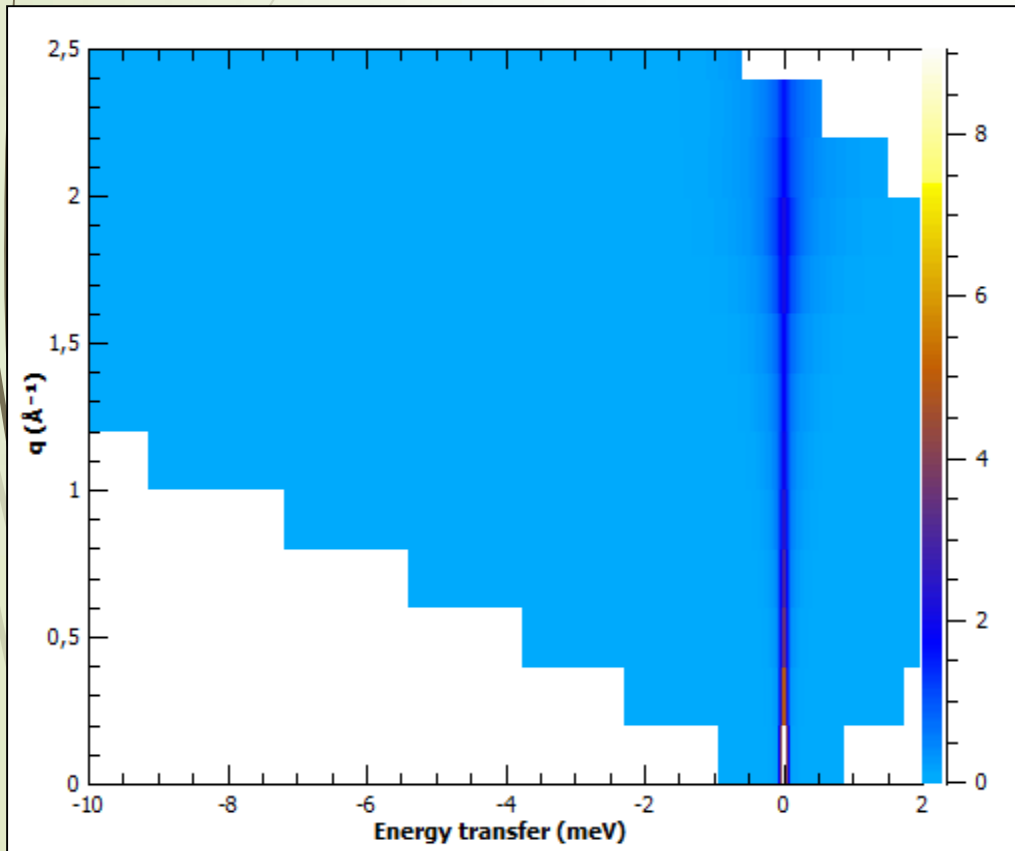
OCPwt sample is monodisperse even at high concentrations

Clear structural change under constant light illumination

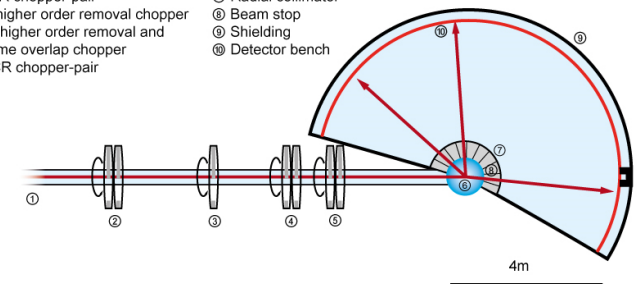


KWS 1 (FRMII)

QENS Measurement under Constant Illumination



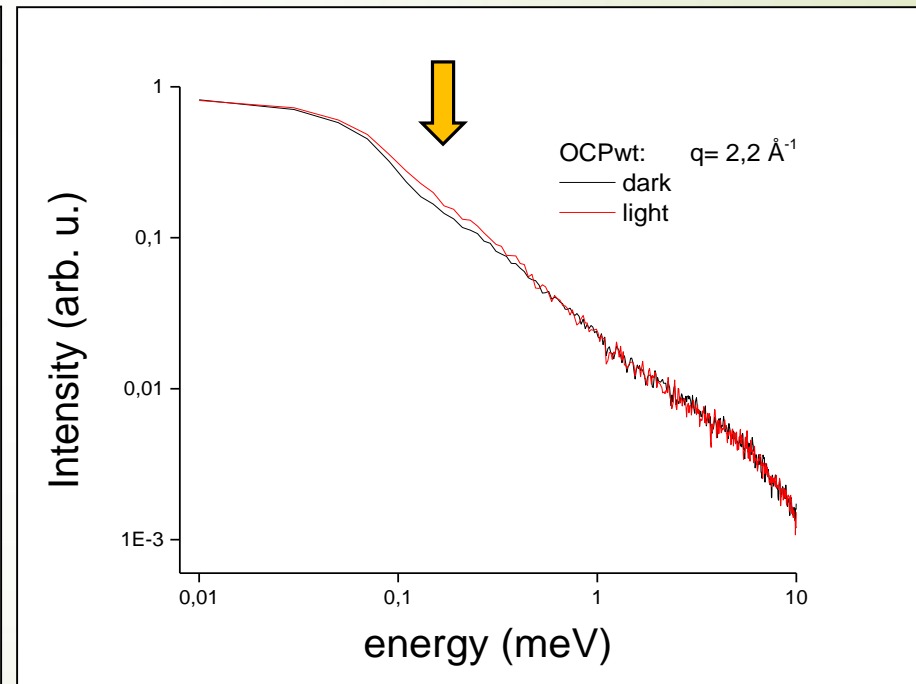
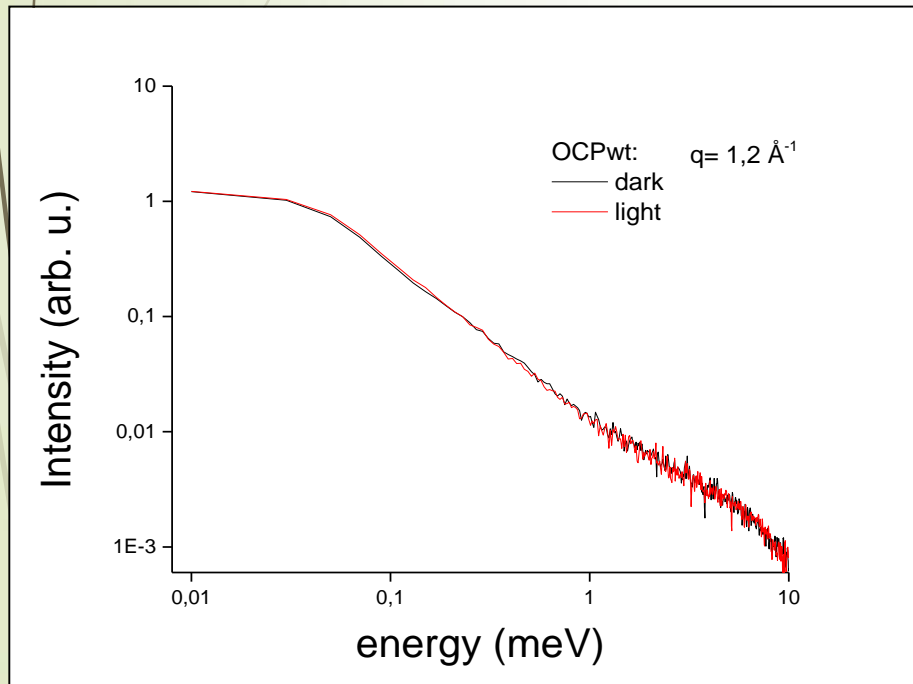
- ① Neutron guide NL2a-u
- ② PCR chopper-pair
- ③ 1st higher order removal chopper
- ④ 2nd higher order removal and frame overlap chopper
- ⑤ MCR chopper-pair
- ⑥ Sample position
- ⑦ Radial collimator
- ⑧ Beam stop
- ⑨ Shielding
- ⑩ Detector bench



Tof_Tof (FRMII)

QENS Light Effect

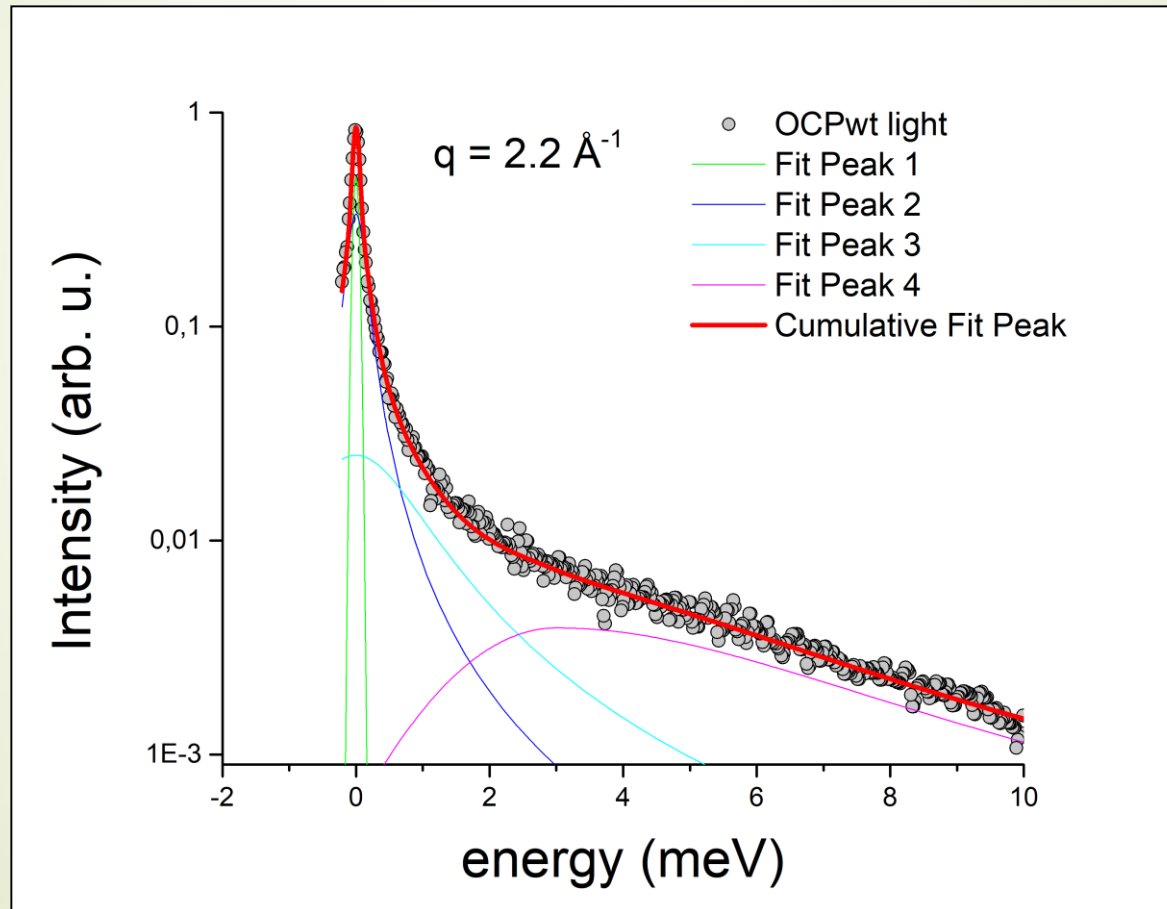
Activation of slow motions



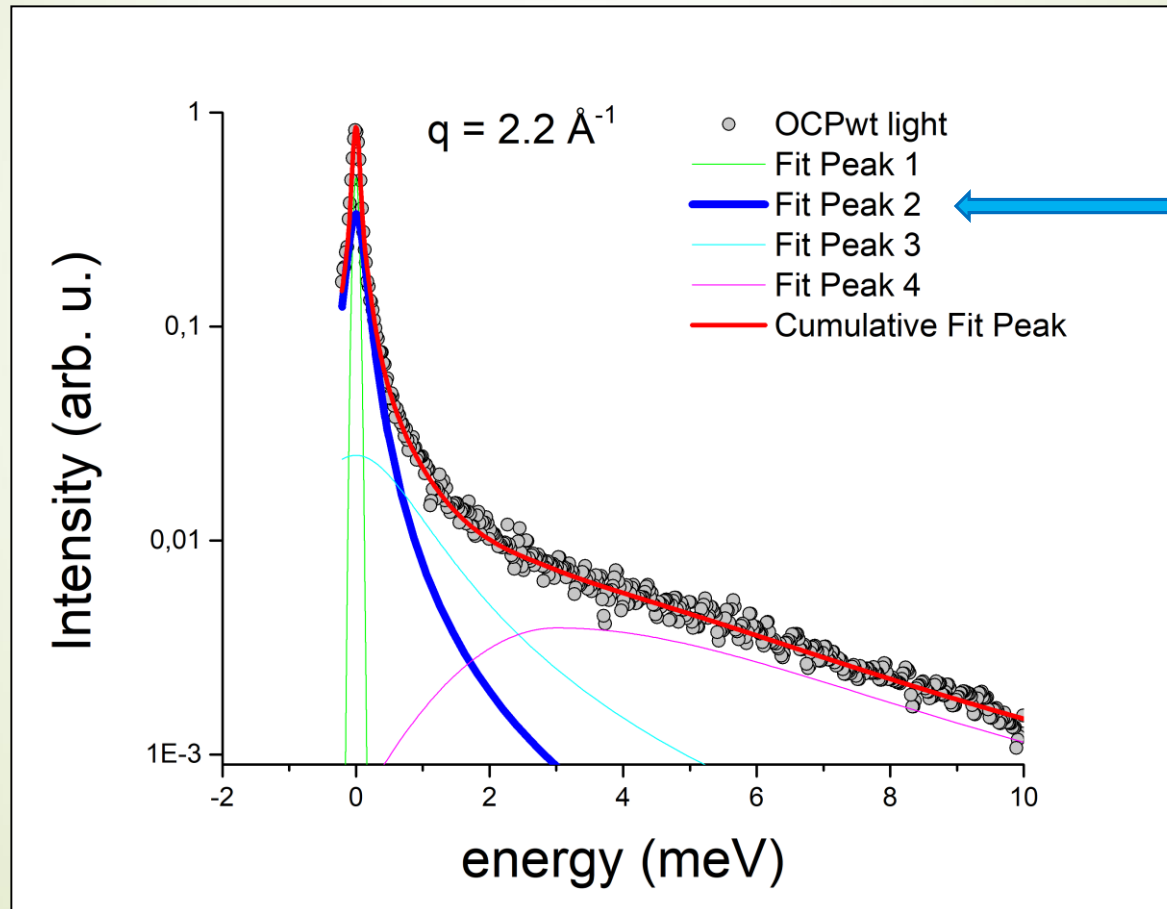
Light effect is seen only
at high q

Tof_Tof (FRMII)

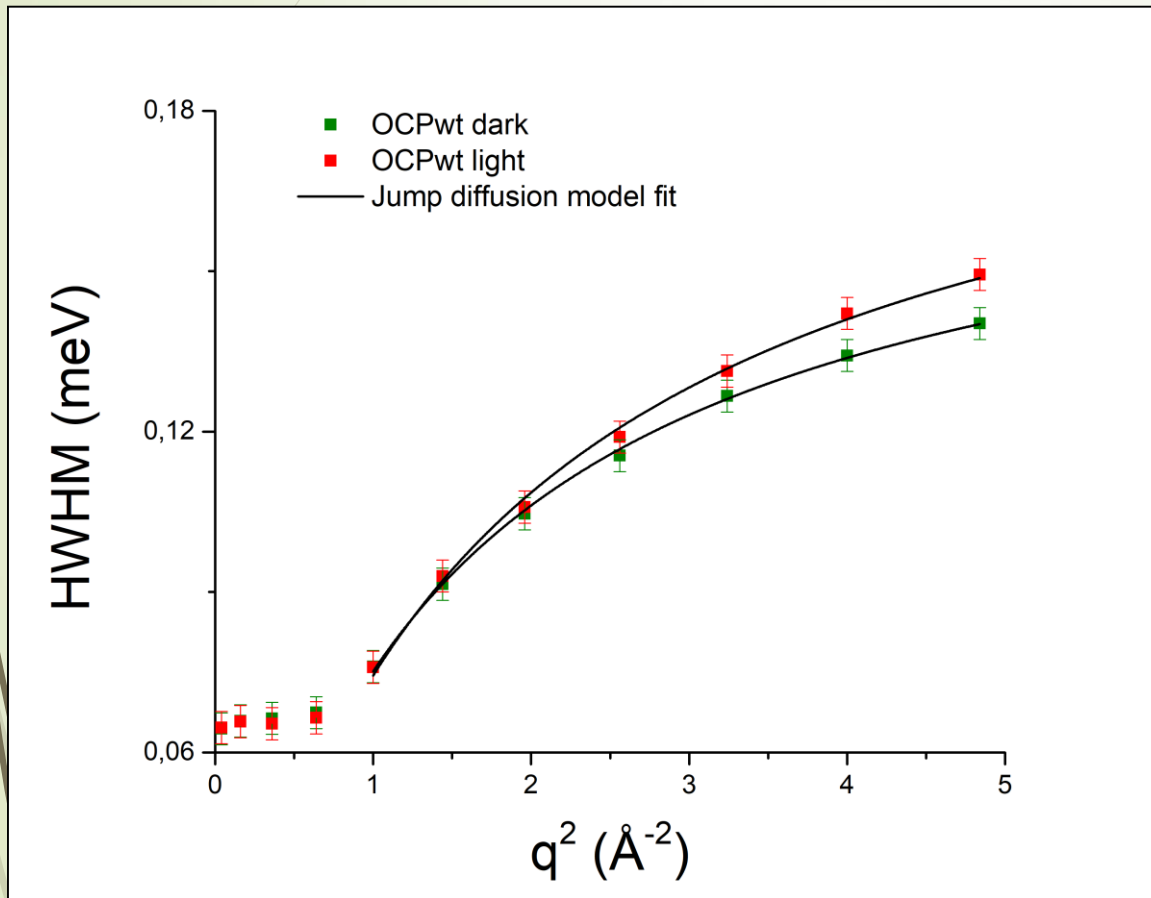
Model Free QENS Data Analysis



Model Free QENS Data Analysis



QENS Light Effect



QENS results:

Under constant light illumination, an additional activation of slow motions occurs

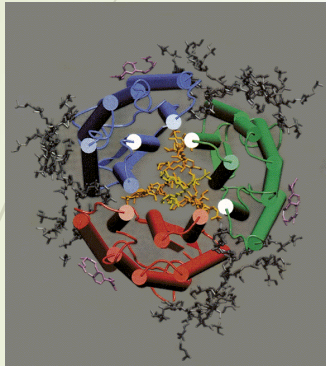
Residence time of molecules is reduced from 3.61 ps to 3.24 ps



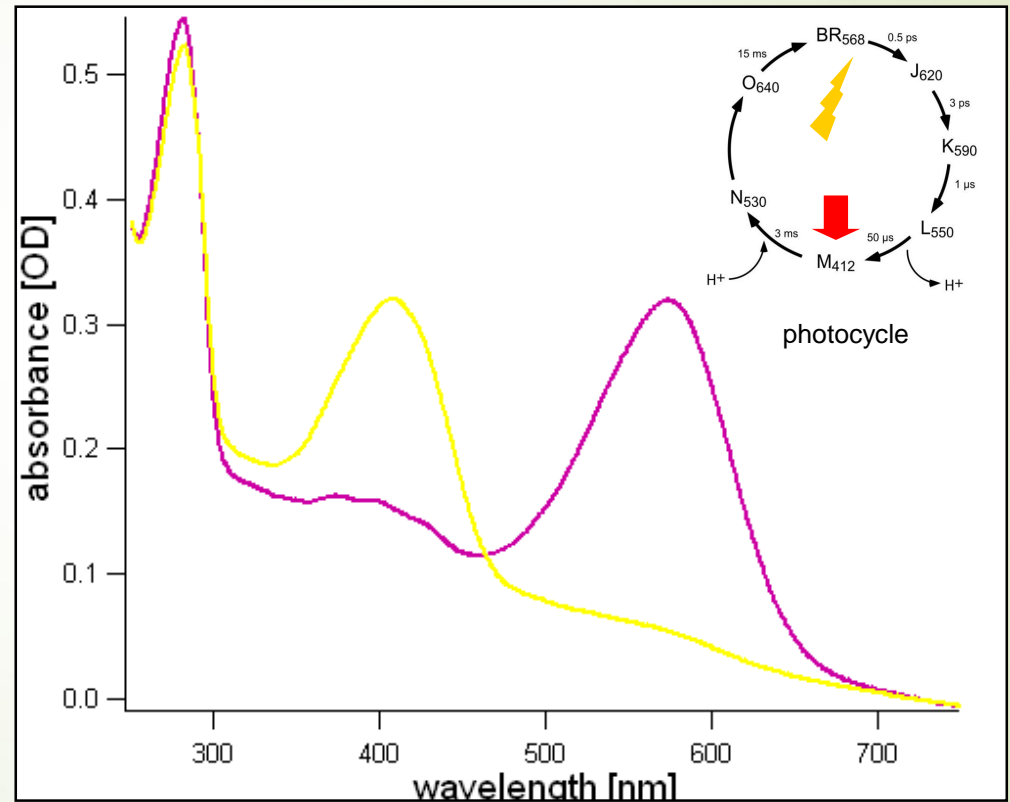
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Time-Resolved QENS experiment Bacteriorhodopsin (BR)

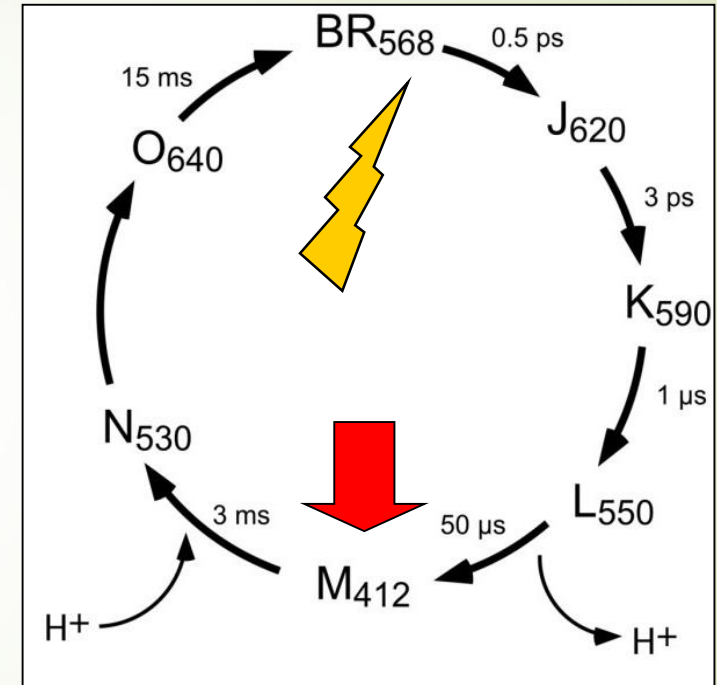
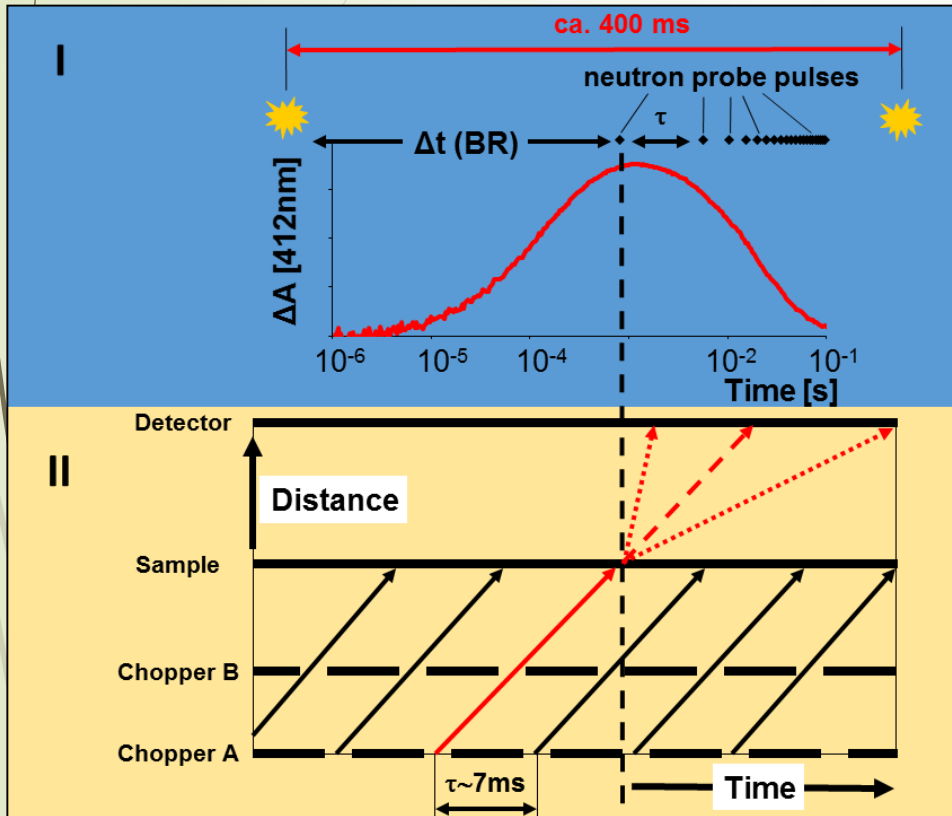


Sass et al., Nature, 2000



M₄₁₂ red-shift of BR absorption due to deprotonation of Schiff's base

Time-Resolved QENS experiment



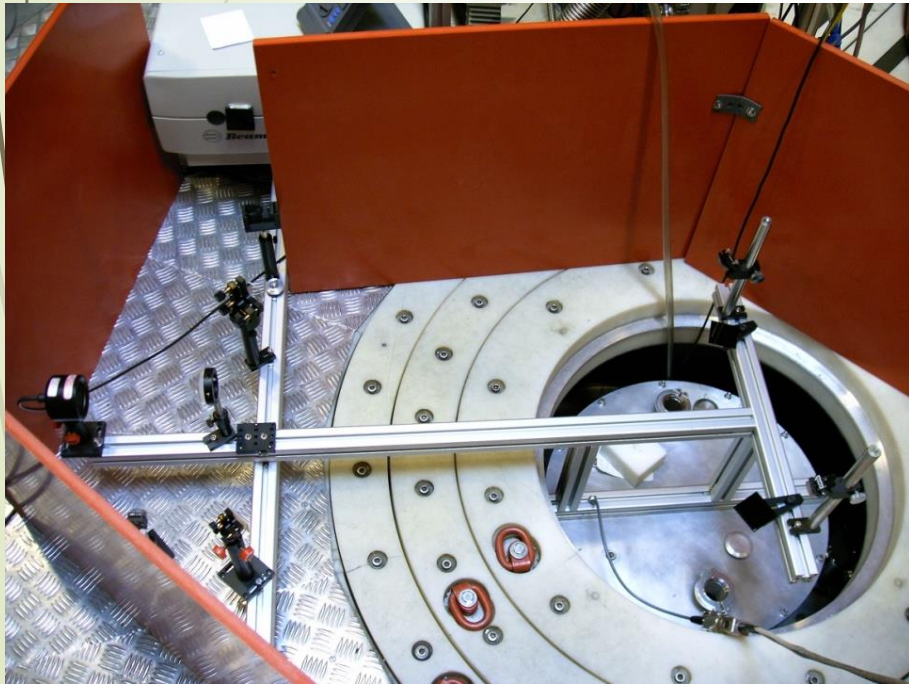
BR photocycle

Neutron pulse is synchronized with the pulsed laser excitation

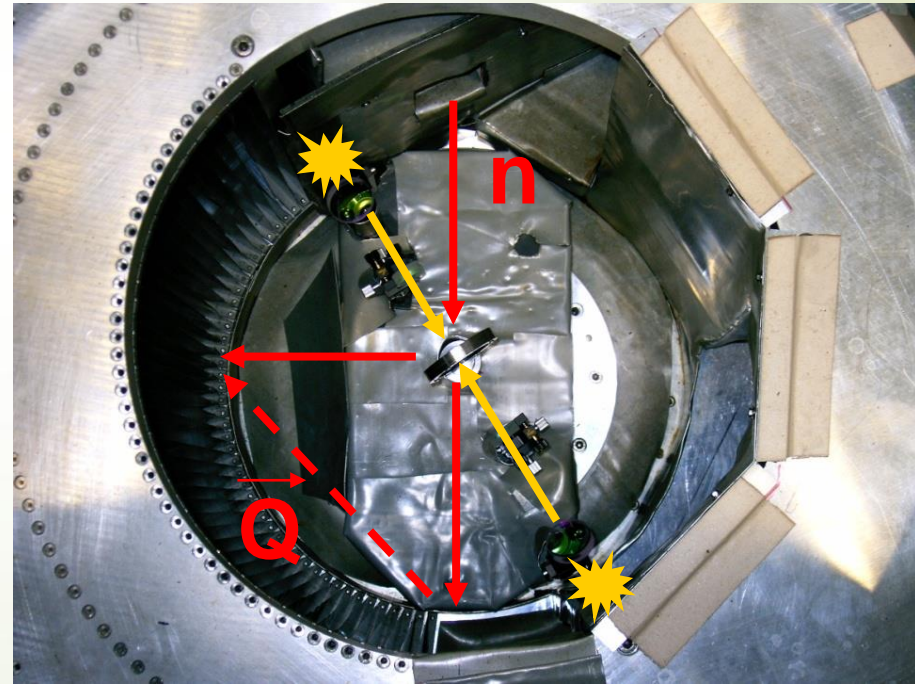
IN5 (ILL)

Laser Setup at IN5 and NEAT Instruments

Sample chamber

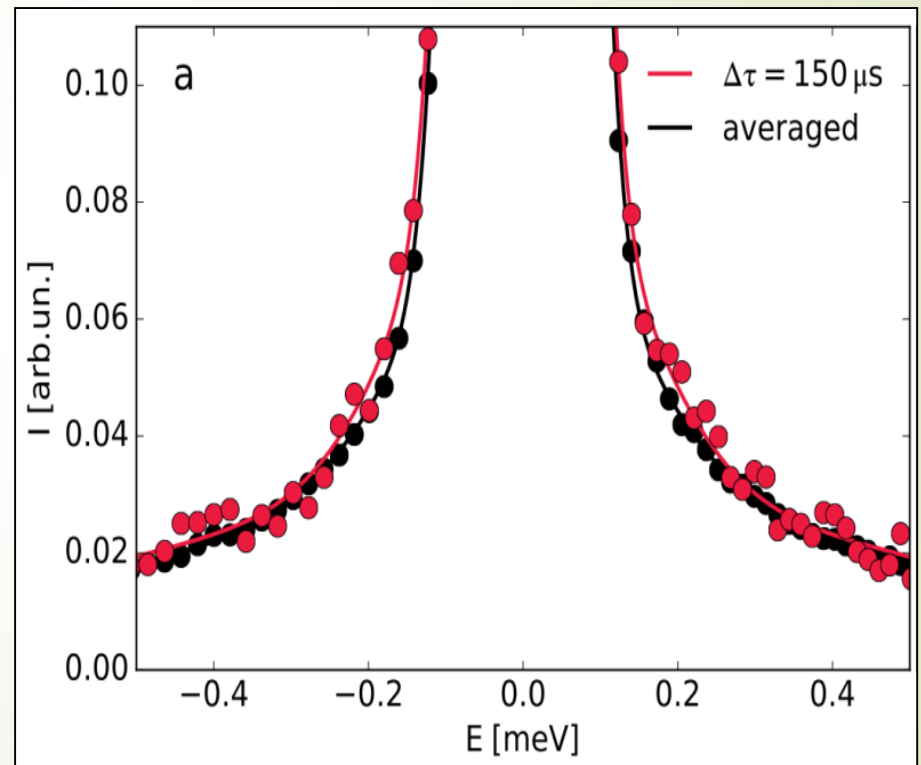
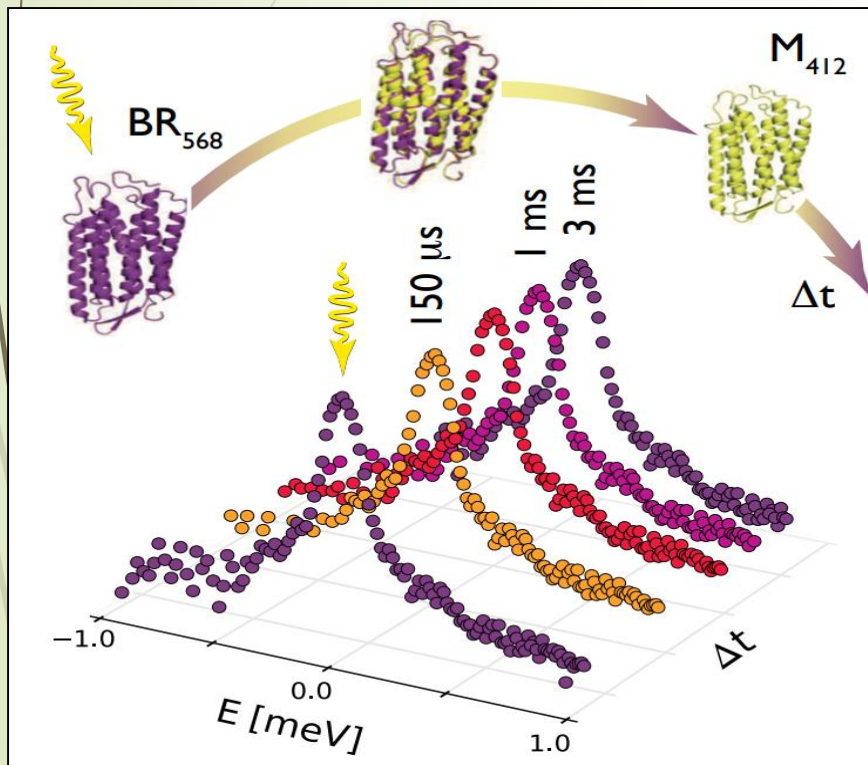


Instrument platform

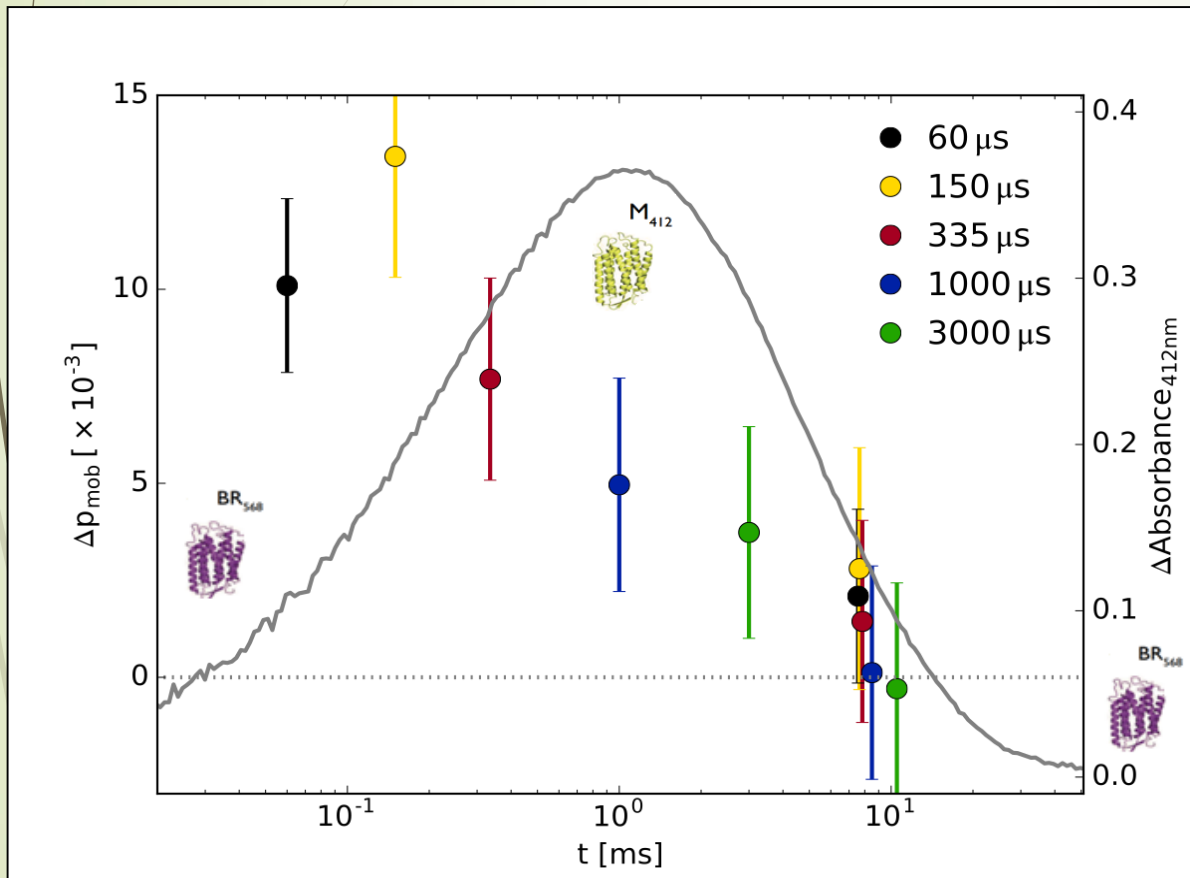


IN5 (ILL)

Time-Resolved QENS



Time-Resolved QENS Light Effect



QENS results:

Light-modulated protein flexibility is actively involved in functionally relevant processes

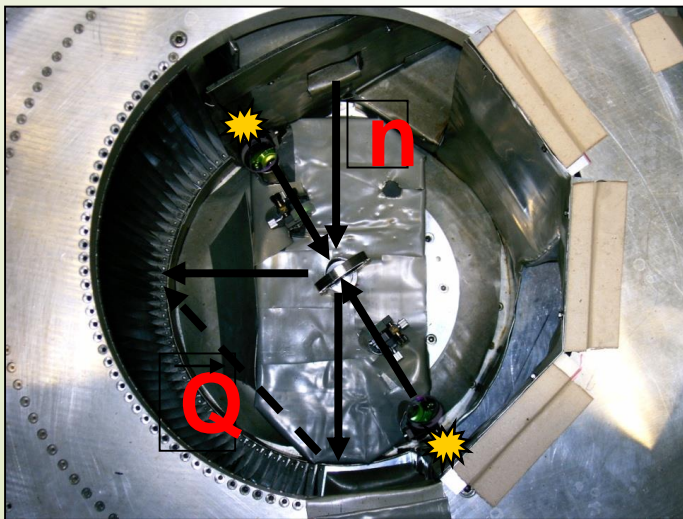
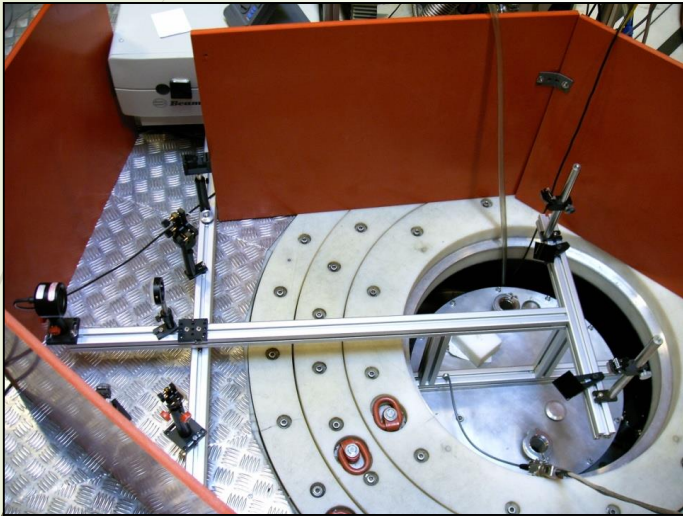
Picosecond fluctuations seems to be a prerequisite to overcome potential energy barriers for the global structural change of BR



Outline

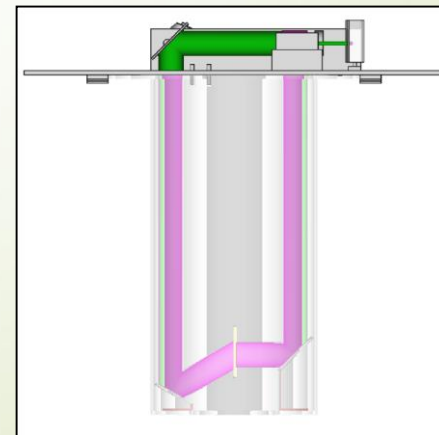
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Concept of pump-probe cell



Needed features of laser setup:

- Light source
- Focusing optic
- Active cooling
- Synchronization option





Conclusions

- Pump-probe experiments are feasible!
- Permit preparation / selection of certain functional states after proper sample characterization
- Time selection leads to large losses in neutron intensity → higher flux needed
- Pump-probe experiments highlight active role of ps-protein dynamics in functional processes



Acknowledgments

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HZB:

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ILL:

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**Thank you for your
attention!!!**

