ADAM MICKIEWICZ
UNIVERSITY
POZNAŃ

Science Applications with XFELs: chemical reactions dynamics

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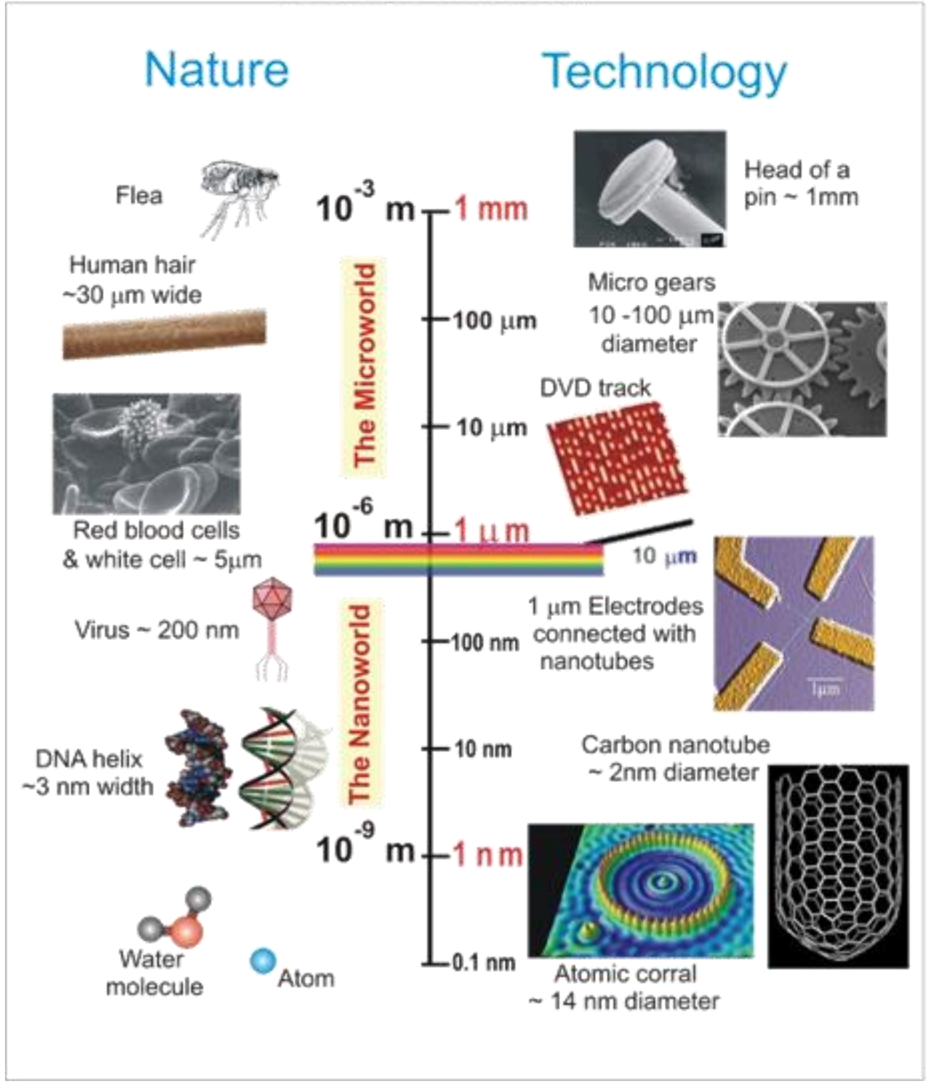
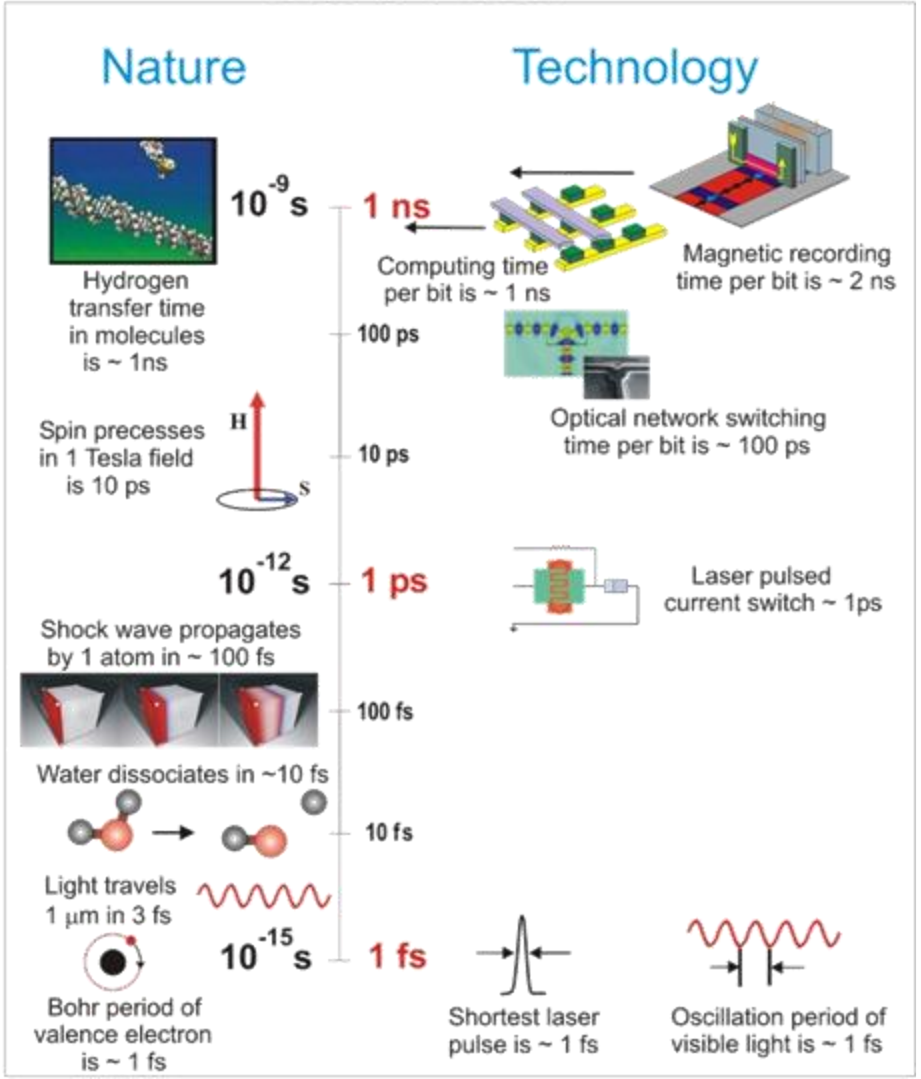
Outline

1. Motivation
2. Short reminder about XAS/XES and WAXS
3. Combining spectroscopy and scattering
4. Examples of chemical dynamics probed with XFELs
5. FXE Instrument at the EuXFEL
6. Conclusions and outlook

Connection between time- and length scales

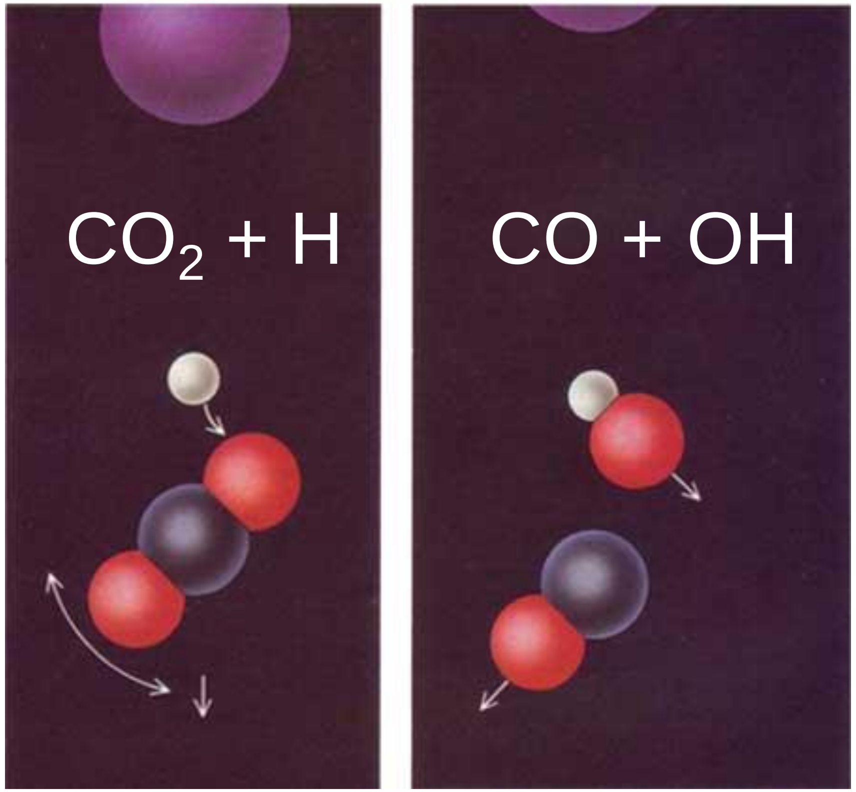




How fast must our camera be?

0.001 s


Hamburg, Bahrenfeld horse track (2011)



Faster than 1 ps =

10^{-12} s, one picosecond

Speed of sound:

1000 m/s => 1.0 Å in 100 fs

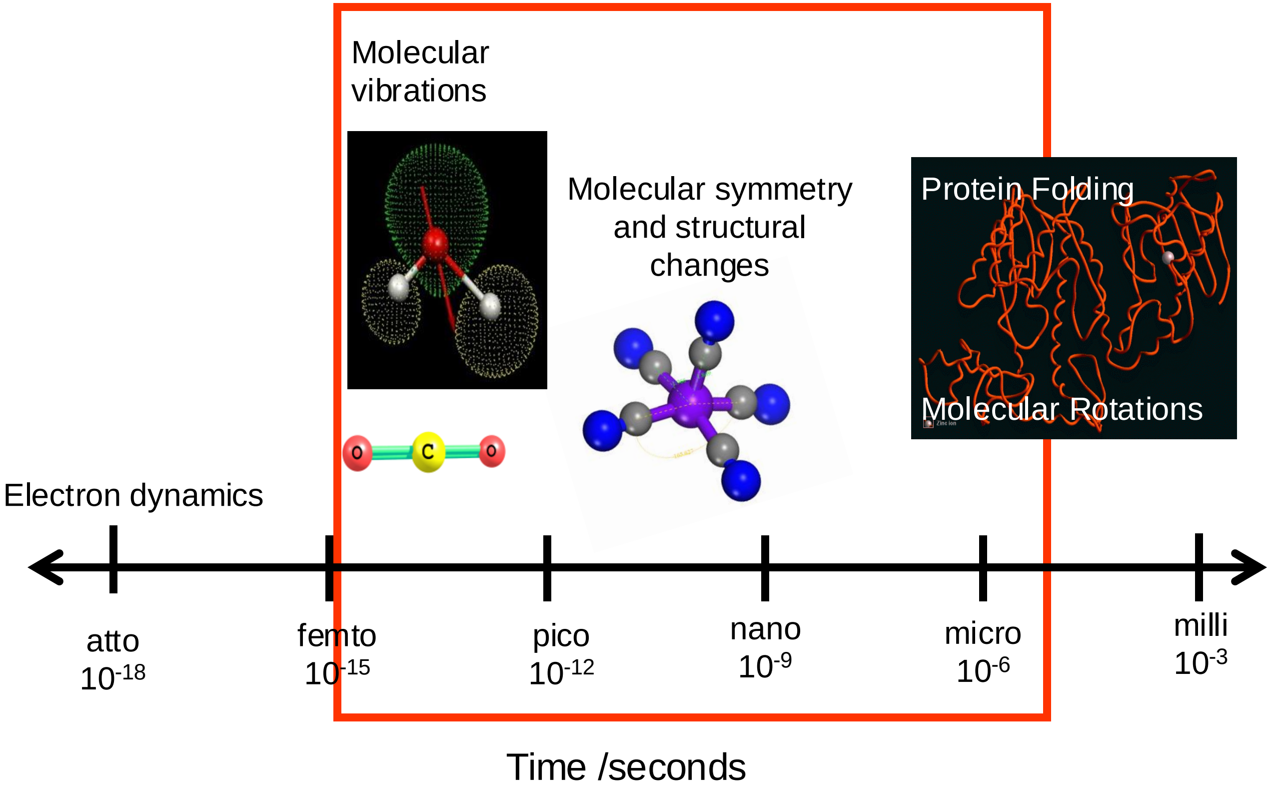
Timescale of half-oscillations of a molecular vibration:

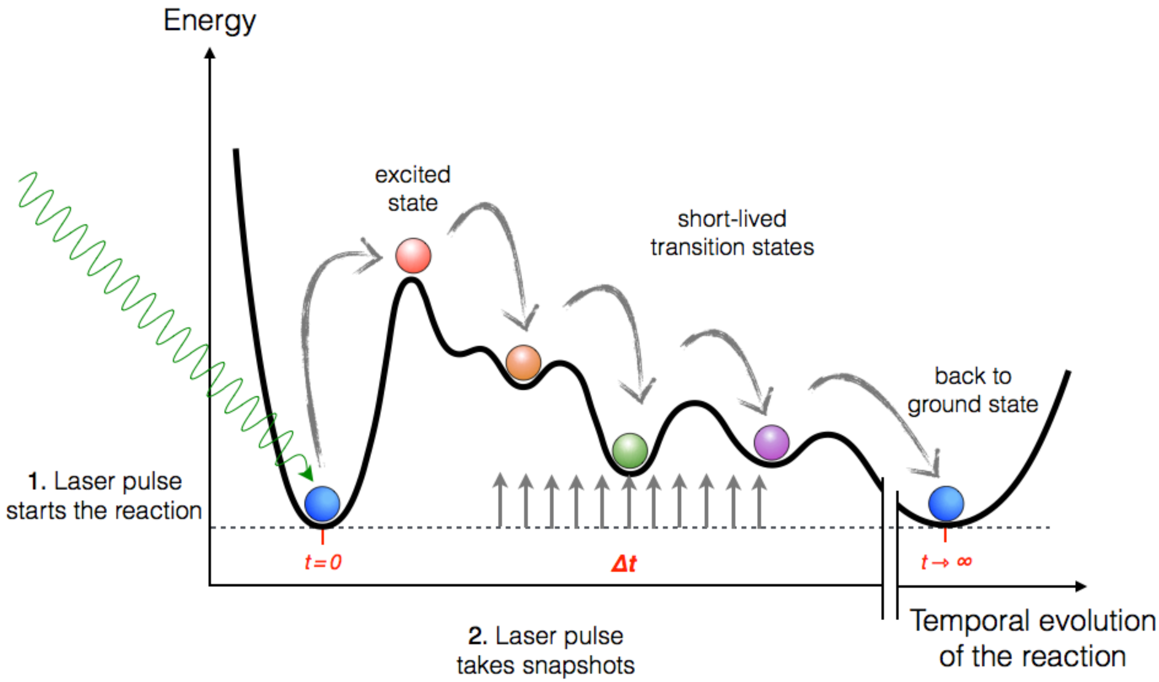
H_2; ω_e= 4155 cm^{-1} → 7.6 fs

I_2; ω_e= 120 cm^{-1} → 270 fs

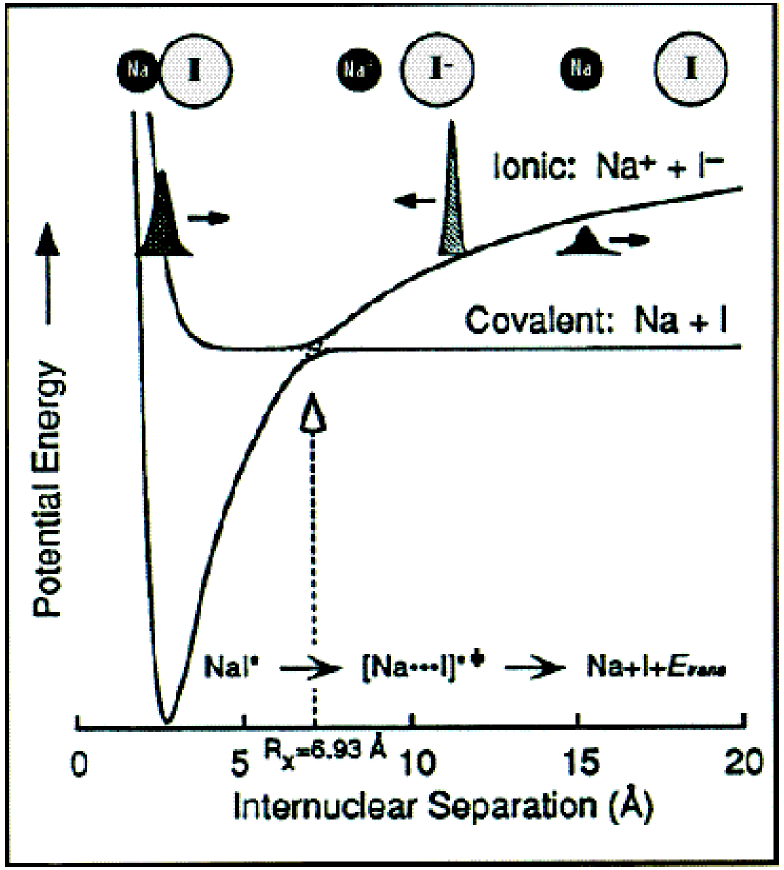
What are the fundamental timescales in Chemistry?

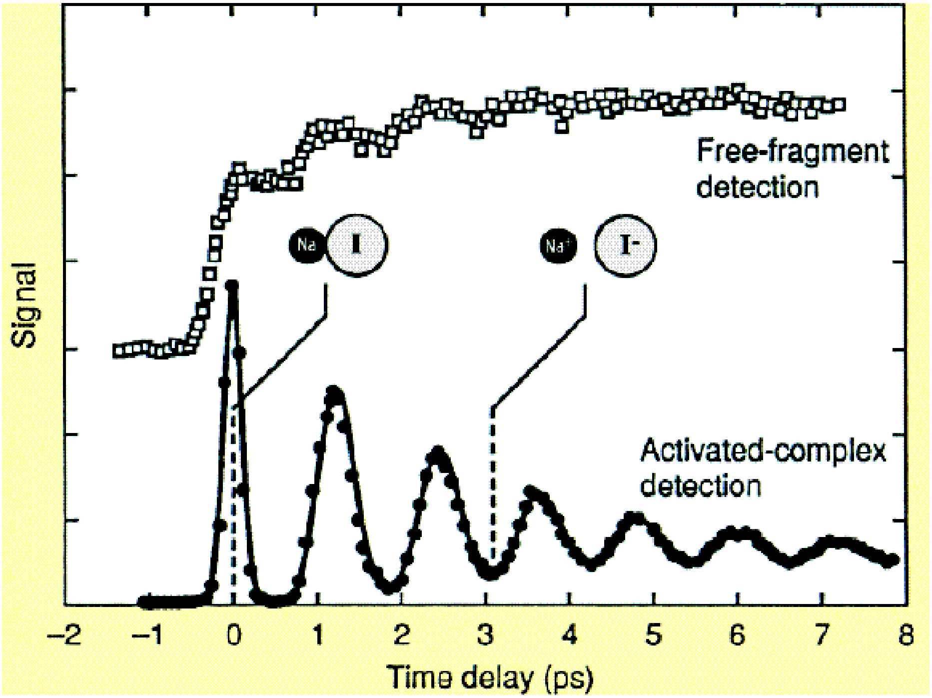
Molecular wavepacket dynamics, bond formation, ligand exchange, photocatalysis, photosynthesis, etc…





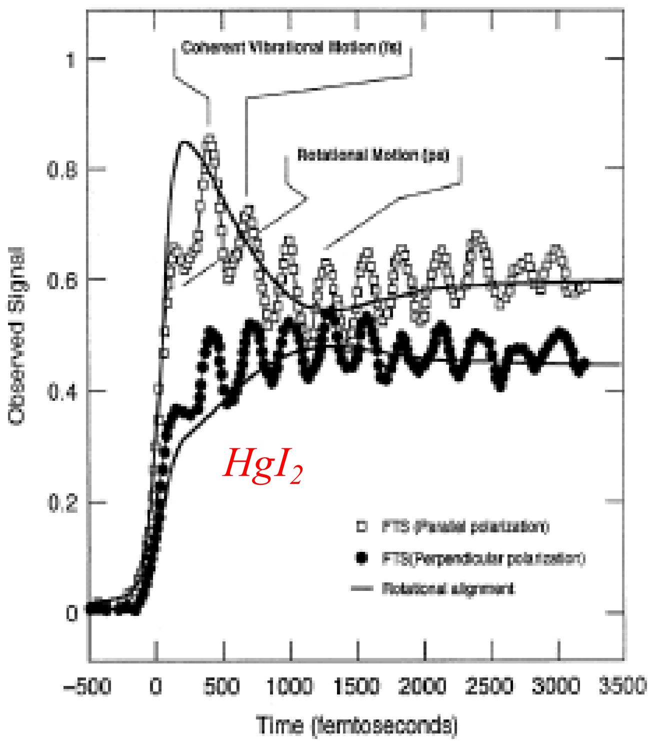
Coherent nuclear dynamics in condensed matter

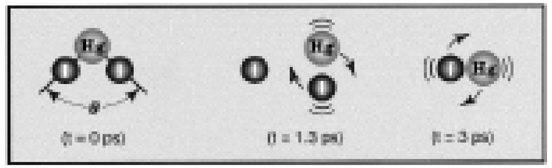




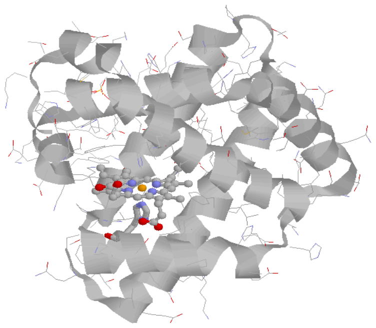
A. H. Zewail et al, J. Phys. Chem. A 104, (1999) 5660

Complex systems: liquids and proteins

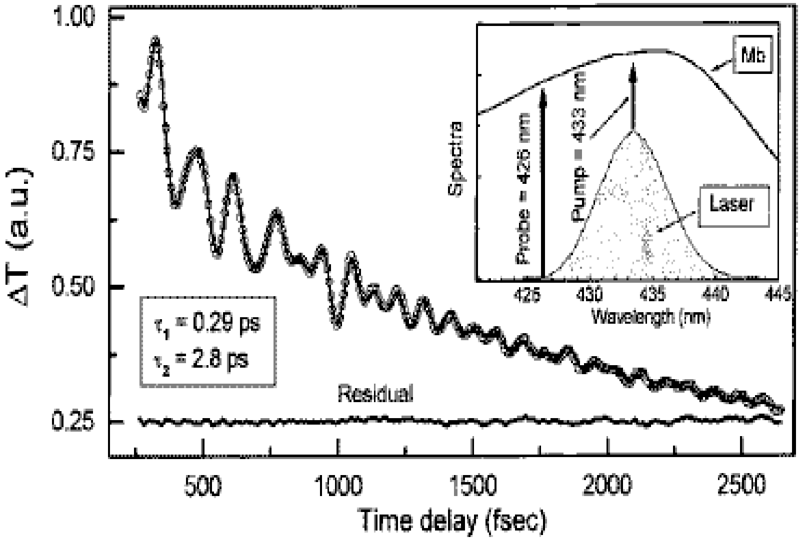




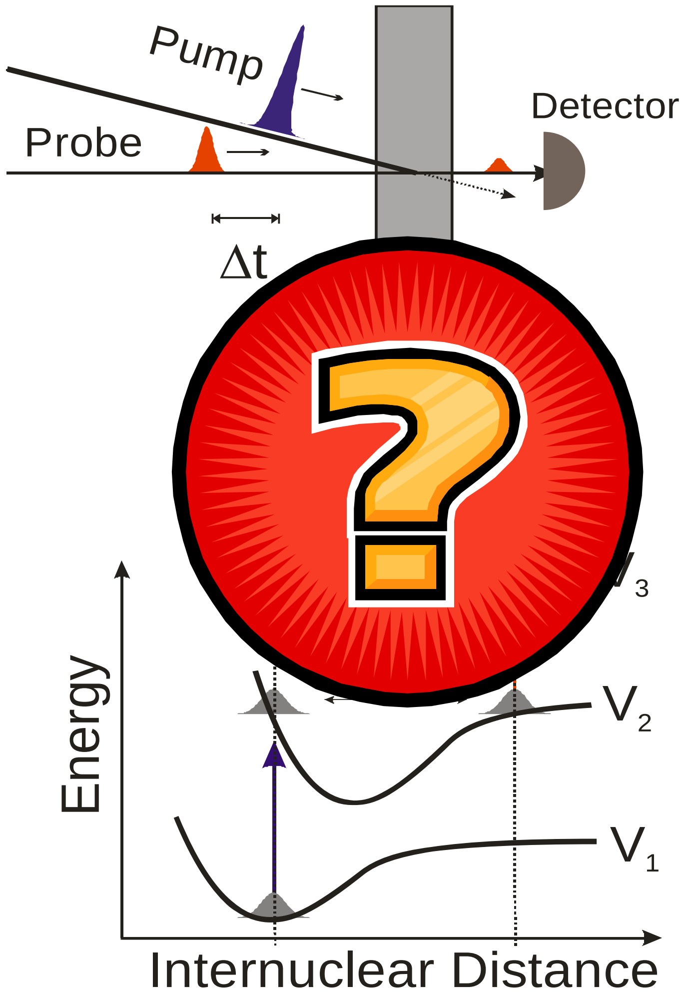
R. Hochstrasser et al, JCP 1993, 1995, 1996

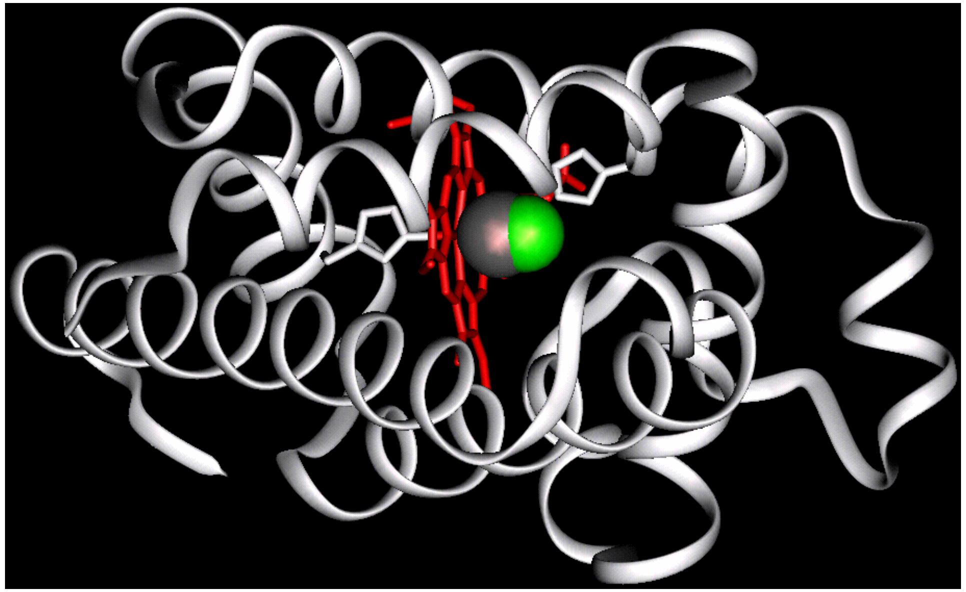


Mb-L



P. Champion et al, JCP 1999, 2000

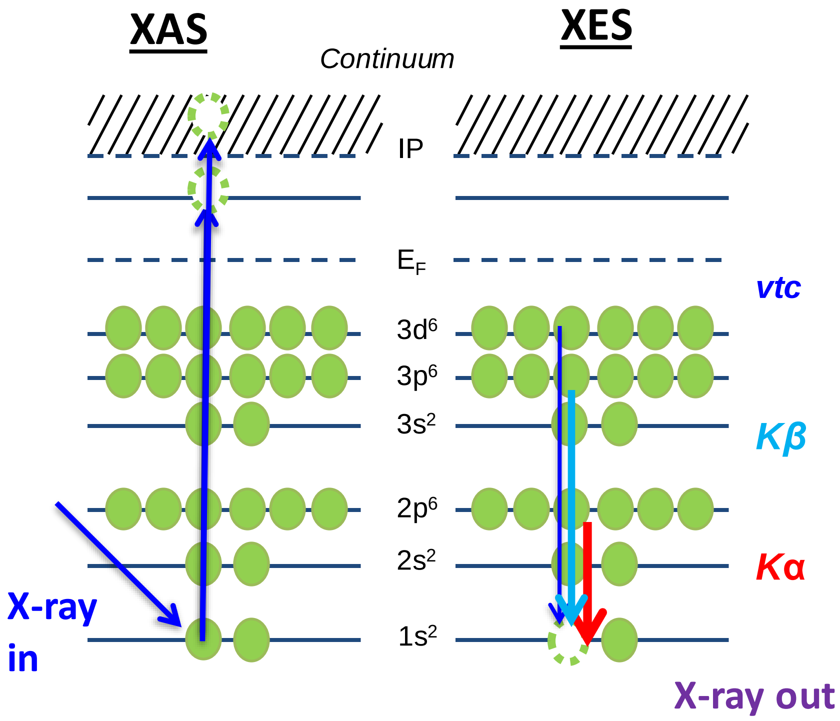


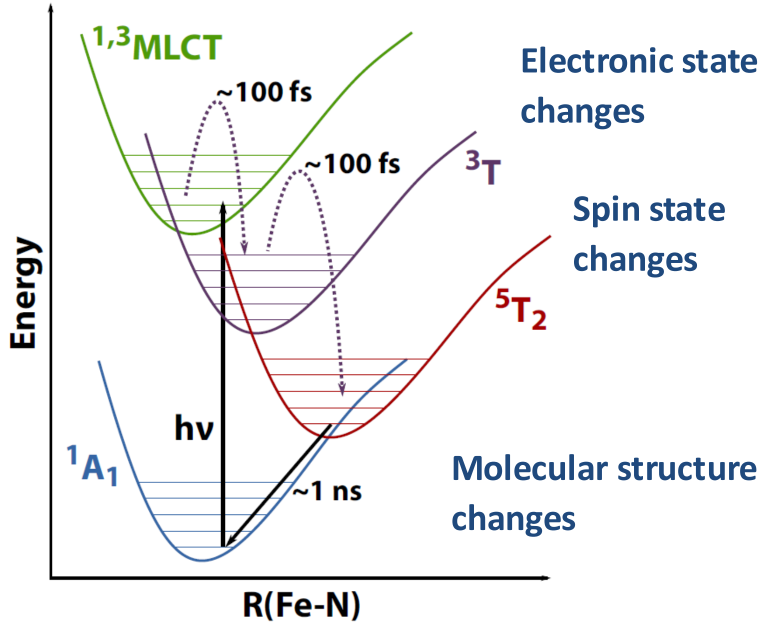


Knowledge of molecular structure becomes inherently difficult when system increases in size!

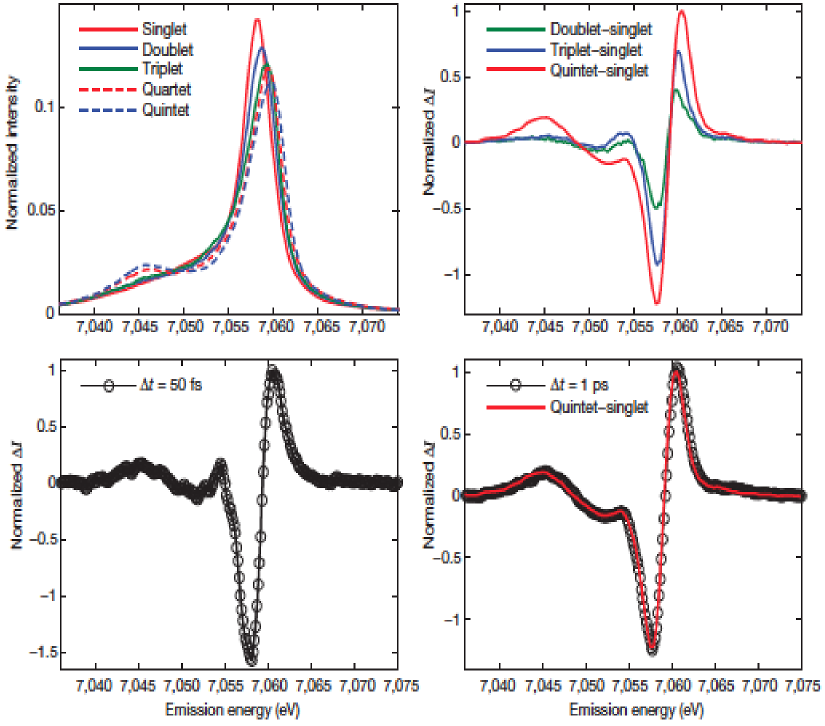
Resolve Atomic Interactions Beyond Optical Wavelengths…

Time-resolved X-ray Spectroscopy





Kβ emission ***on [Fe(bpy)$_3$]$^{2+}$***



W. Zhang *et al.*, Nature, **509** (2014) 345

X-ray Emission Spectroscopy (XES)

Occupied molecular orbitals

Spin State

X-ray Absorption Spectroscopy (XAS)

Unoccupied molecular orbitals

Molecular structure

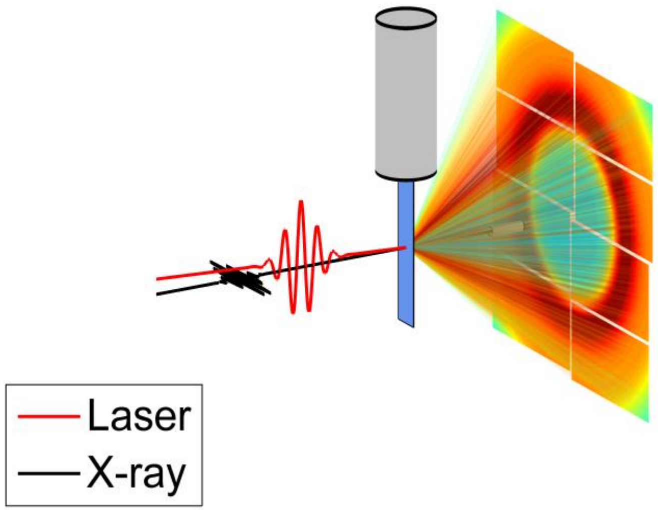
Oxidation state

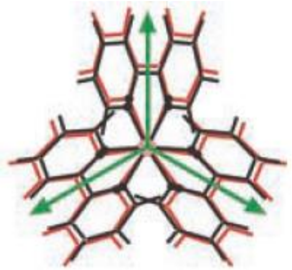
Element specific

Time-resolved X-ray scattering in liquids (WAXS)

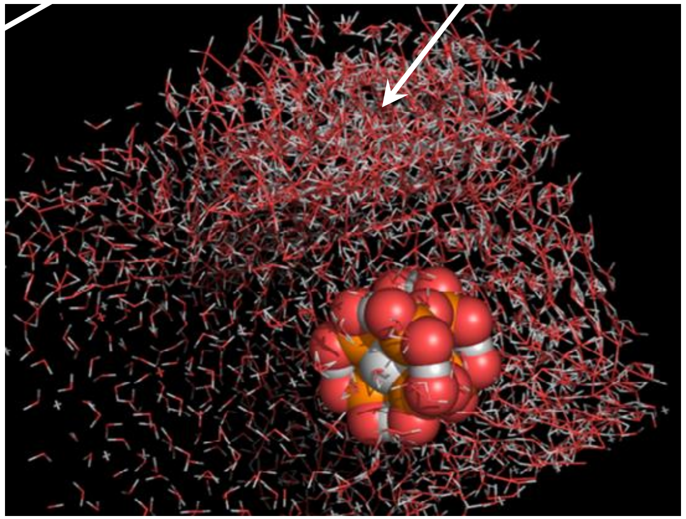
Transient XDS signal arise from the structural changes in:

$$\Delta S(Q, \Delta t) = \Delta S_{solute} + \Delta S_{solvent} + \Delta S_{cage}$$

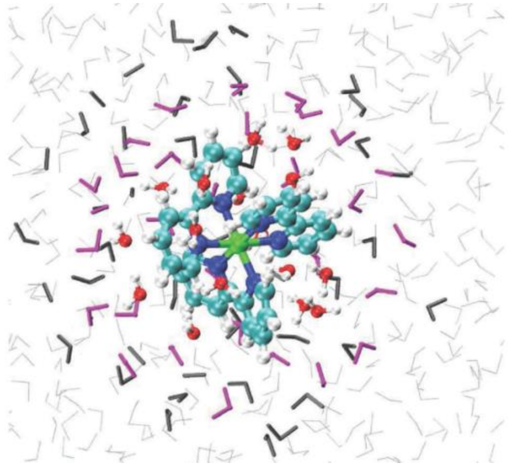




Solute Structure



Bulk Solvent



Solute-solvent interaction
(”solvation shell”/cage)

$$\Delta S_{Calc} = \alpha \Delta S_{Solute} + \Delta T \left.\frac{\partial \Delta S}{\partial T}\right|_{\rho} + \Delta \rho \left.\frac{\partial \Delta S}{\partial \rho}\right|_{T}$$

Time-resolved X-ray scattering in liquids (WAXS)

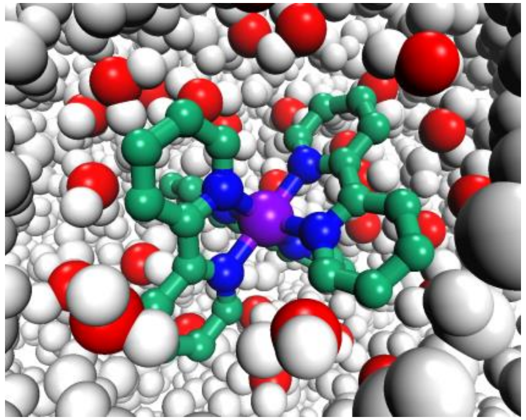
$$\Delta S(Q,t) = \Delta S_{solute}(Q,t) + \Delta S_{cage}(Q,t) + \Delta S_{solvent}(Q,t)$$

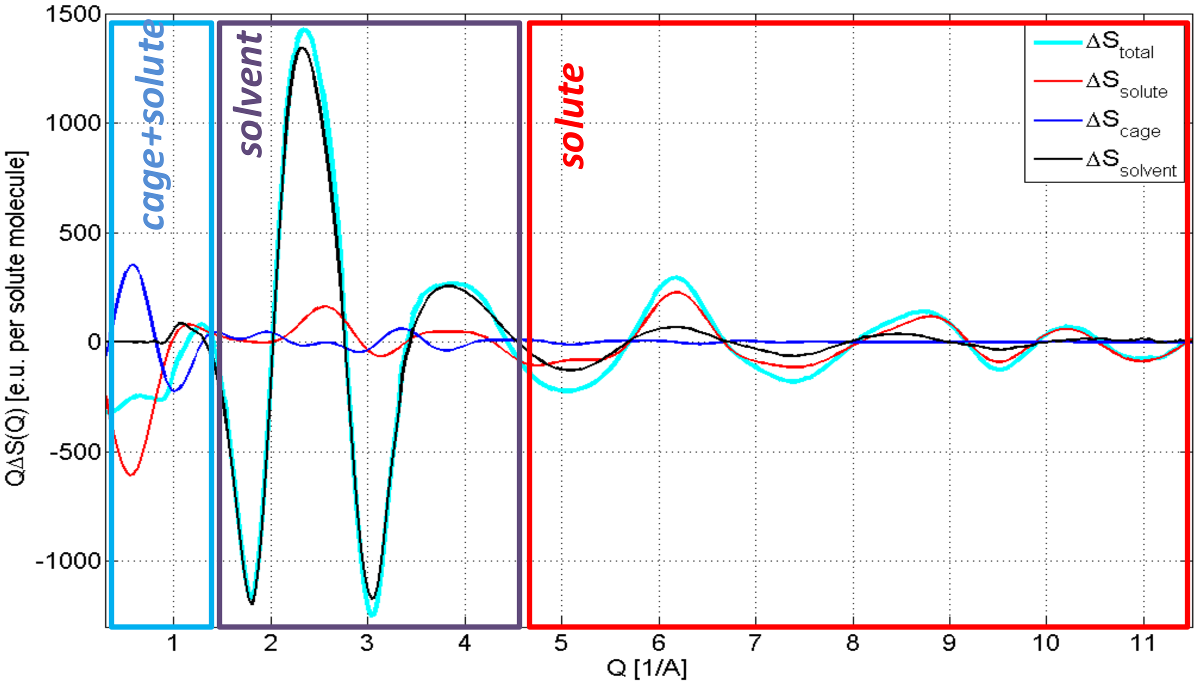
where: $$\Delta S_{solvent}(Q,t) = (\frac{\partial S_{solv}(Q)}{\partial T} \cdot \Delta T(t) + \frac{\partial S_{solv}(Q)}{\partial \rho} \cdot \Delta \rho(t))$$

Solute term: $$S_{solute}(Q) = \sum_n f_n^2(Q) + \sum_n \sum_{m \neq n} (f_n(Q) \cdot f_m(Q) \cdot \frac{sin(Q \cdot r_{nm})}{Q \cdot r_{nm}})$$

Solvation cage term: $$S_{cage}(Q) = \sum_n N_n f_n^2(Q) + \sum_n \sum_{m \neq n} (\frac{N_n N_m}{V} f_n(Q) \cdot f_m(Q) \int_0^\infty (g_{nm}(r) - 1) \cdot \frac{sin(Q \cdot r)}{Q \cdot r} \cdot 4\pi r^2 dr)$$

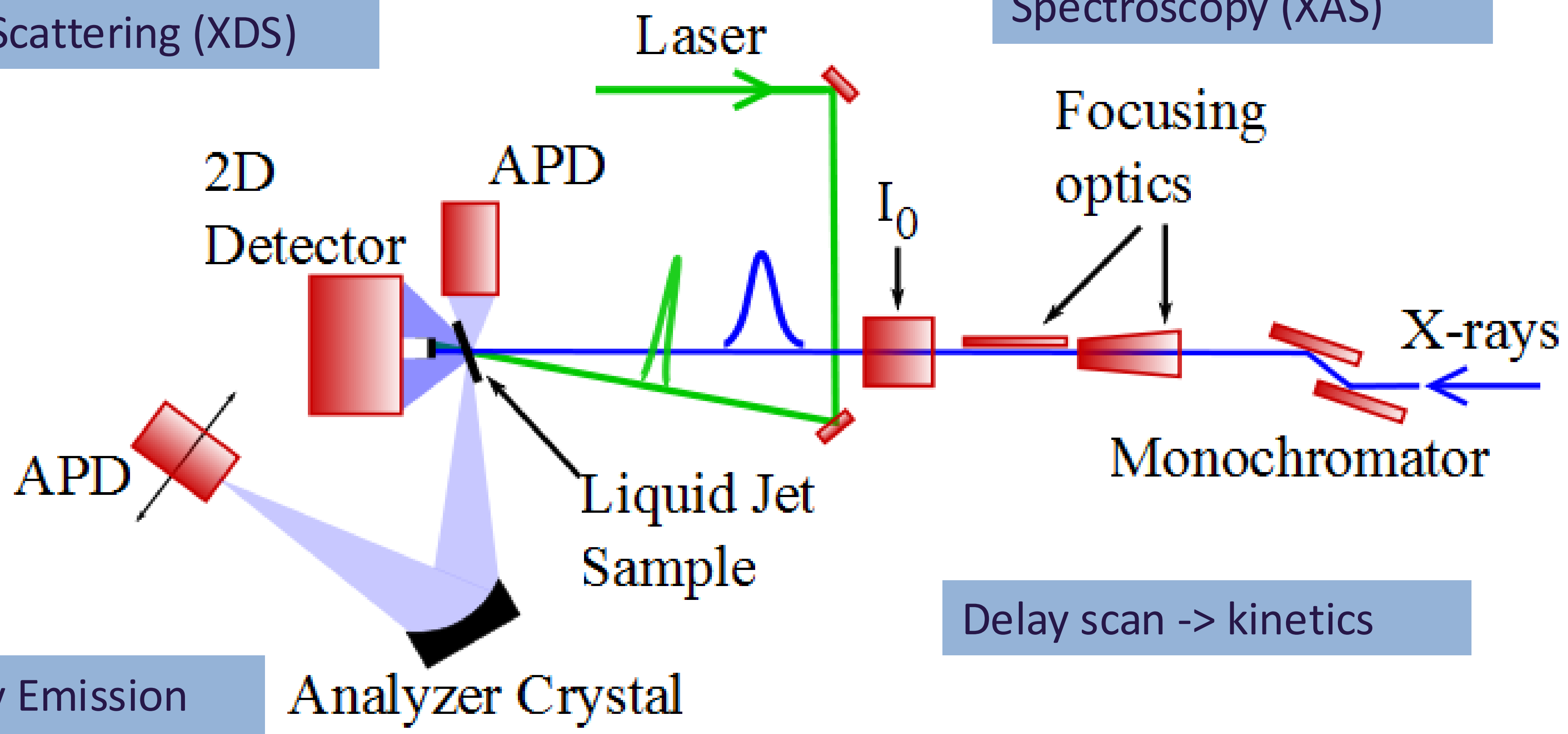
Aqueous [Fe(bpy)$_3$]$^{2+}$





X-ray Diffuse Scattering (XDS)

X-ray Absorption Spectroscopy (XAS)

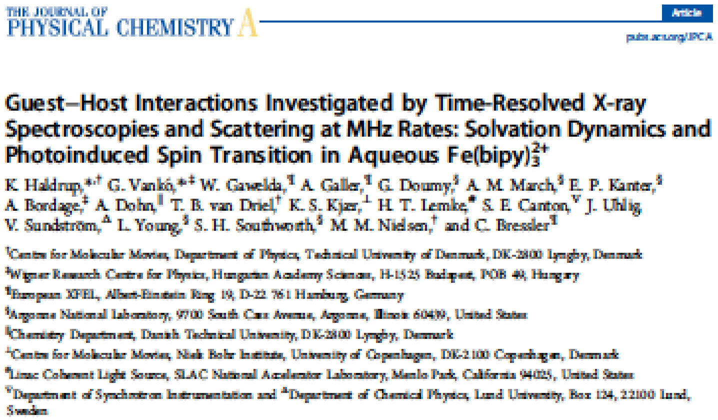


Delay scan -> kinetics

X-ray Emission Spectroscopy (XES)

Combine complementary tools in a single experiment!!

Combining X-ray spectroscopy and scattering (100 ps)



THE JOURNAL OF PHYSICAL CHEMISTRY A

Article

pubs.acs.org/JPCA

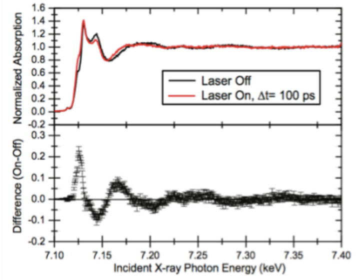
Guest–Host Interactions Investigated by Time-Resolved X-ray Spectroscopies and Scattering at MHz Rates: Solvation Dynamics and Photoinduced Spin Transition in Aqueous $Fe(bipy)_3^{2+}$

K. Haldrup,*,† G. Vankó,*,‡ W. Gawelda,¶ A. Galler,¶ G. Doumy,§ A. M. March,§ E. P. Kanter,§ A. Bordage,‡ A. Dohn,∥ T. B. van Driel,† K. S. Kjær,⊥ H. T. Lemke,# S. E. Canton,∇ J. Uhlig, V. Sundström,△ L. Young,§ S. H. Southworth,§ M. M. Nielsen,† and C. Bressler¶

†Centre for Molecular Movies, Department of Physics, Technical University of Denmark, DK-2800 Lyngby, Denmark
‡Wigner Research Centre for Physics, Hungarian Academy Sciences, H-1525 Budapest, POB 49, Hungary
¶European XFEL, Albert-Einstein Ring 19, D-22 761 Hamburg, Germany
§Argonne National Laboratory, 9700 South Cass Avenue, Argonne, Illinois 60439, United States
∥Chemistry Department, Danish Technical University, DK-2800 Lyngby, Denmark
⊥Centre for Molecular Movies, Niels Bohr Institute, University of Copenhagen, DK-2100 Copenhagen, Denmark
#Linac Coherent Light Source, SLAC National Accelerator Laboratory, Menlo Park, California 94025, United States
∇Department of Synchrotron Instrumentation and △Department of Chemical Physics, Lund University, Box 124, 22100 Lund, Sweden

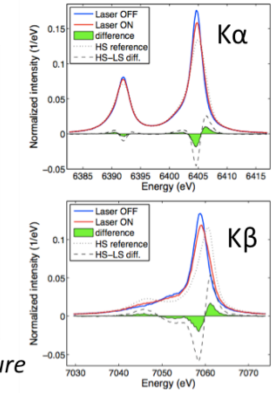
EXAFS yields change in bond length

X-ray absorption spectroscopy



-electronic and geometric structure

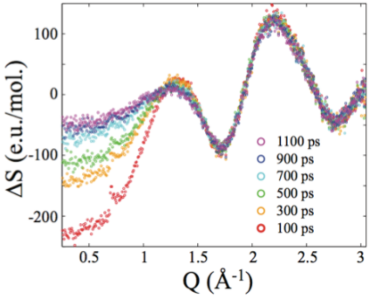
X-ray emission spectroscopy



-direct probe of spin state

Yields excited state geometric structure

X-ray diffuse scattering

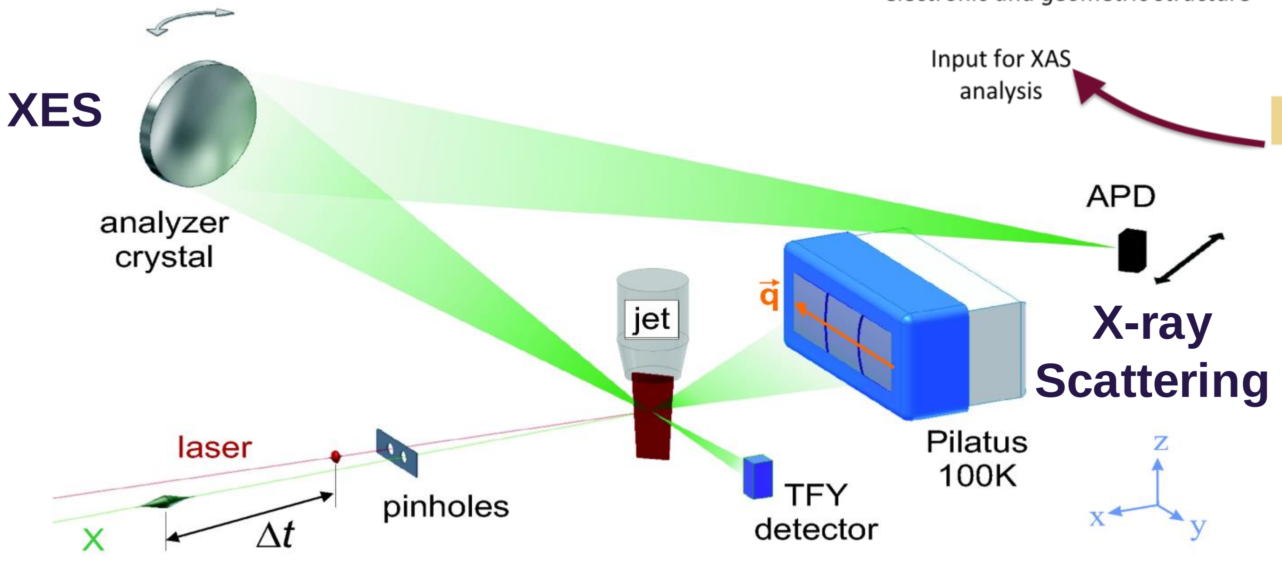


-insight into solvent shell rearrangements

Input for XAS analysis

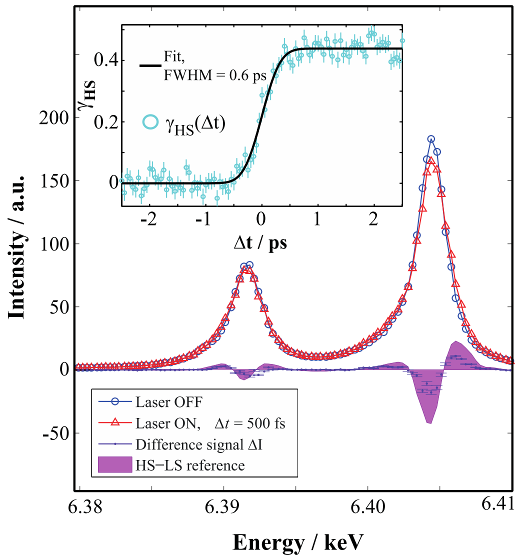
Excited state fraction

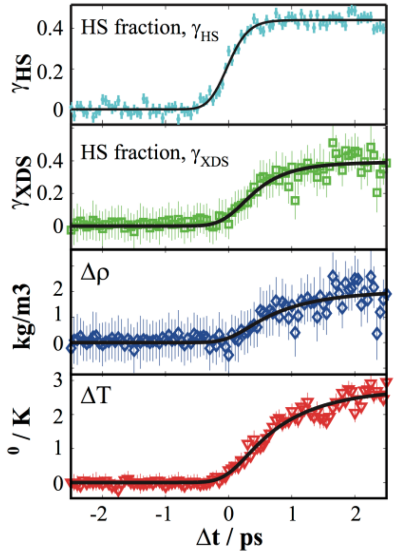
Input for scattering analysis

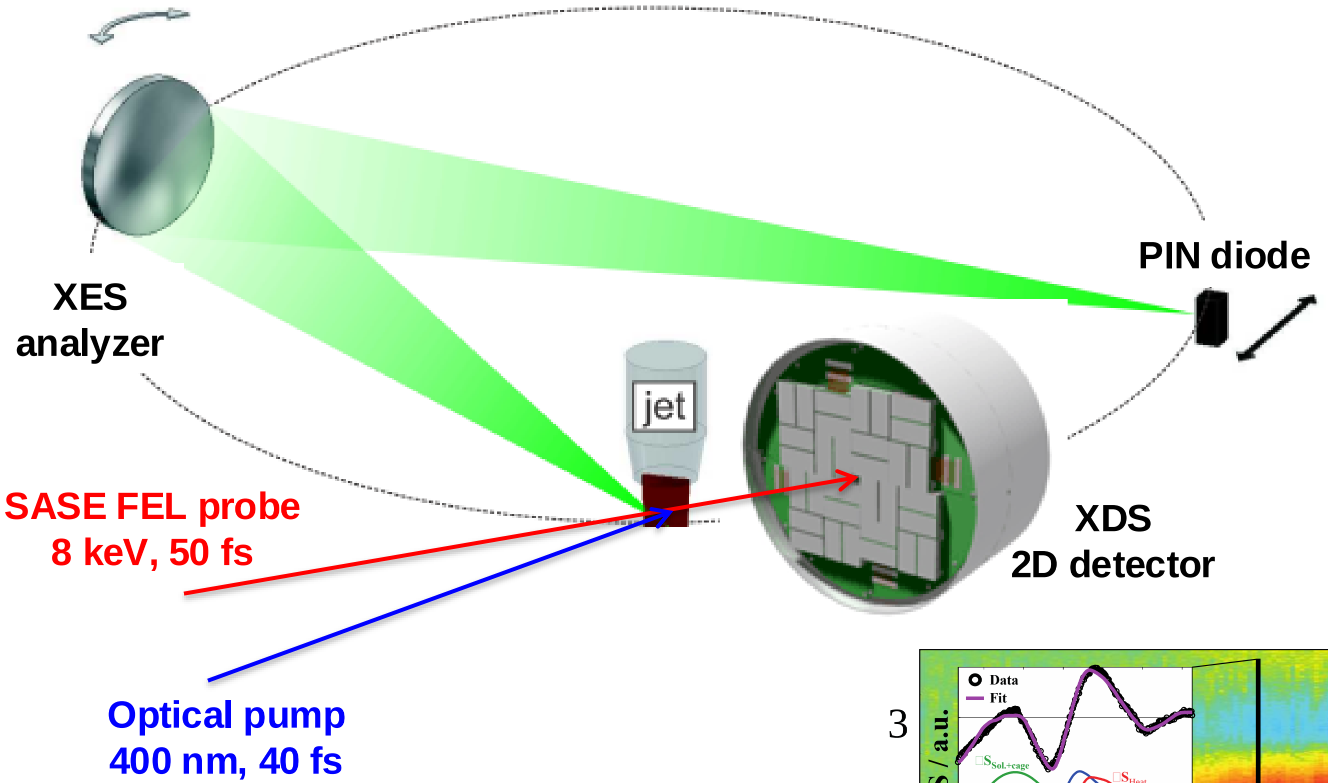


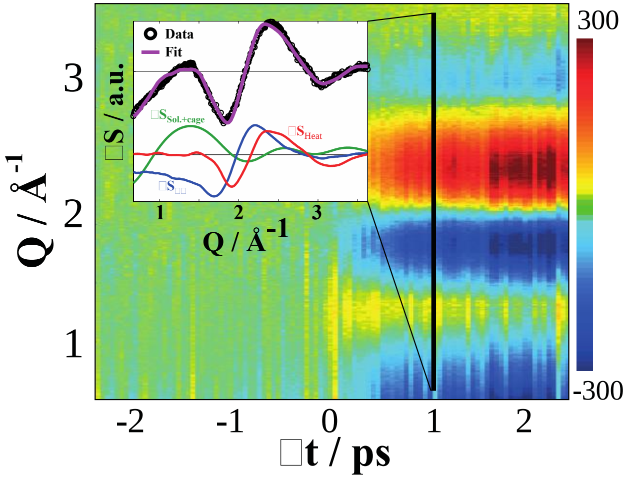
K. Haldrup, W. Gawelda et al., J. Phys. Chem. A (2012)

Combining X-ray spectroscopy and scattering (< 1 ps)



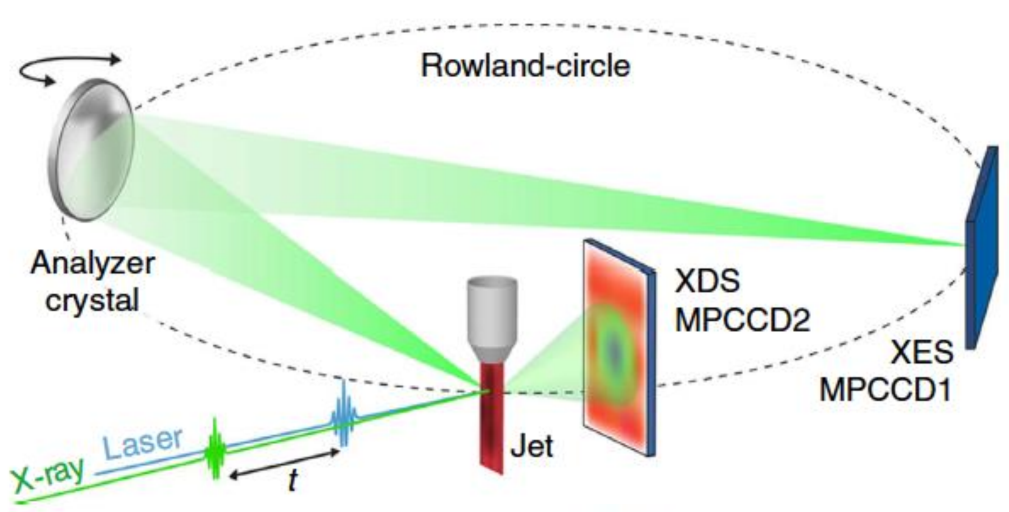


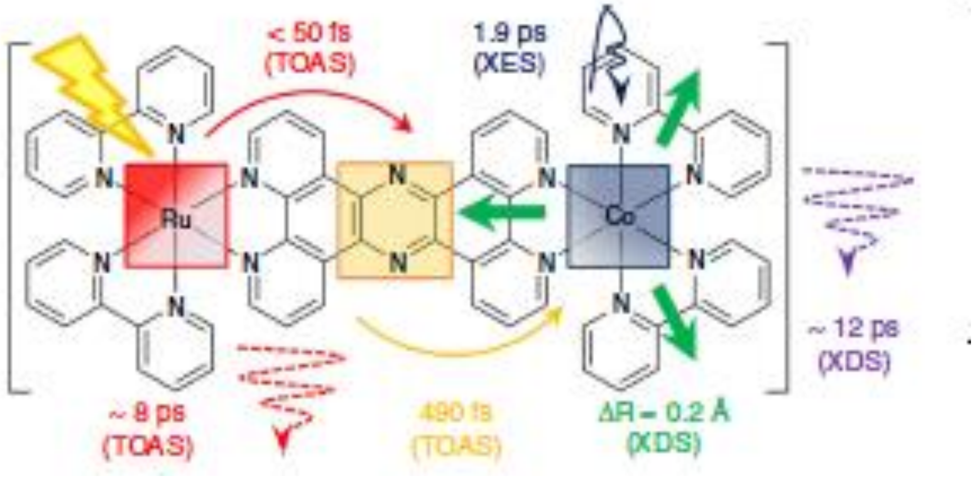




K. Haldrup, W. Gawelda, et al.,
J. Phys. Chem. B (2016)

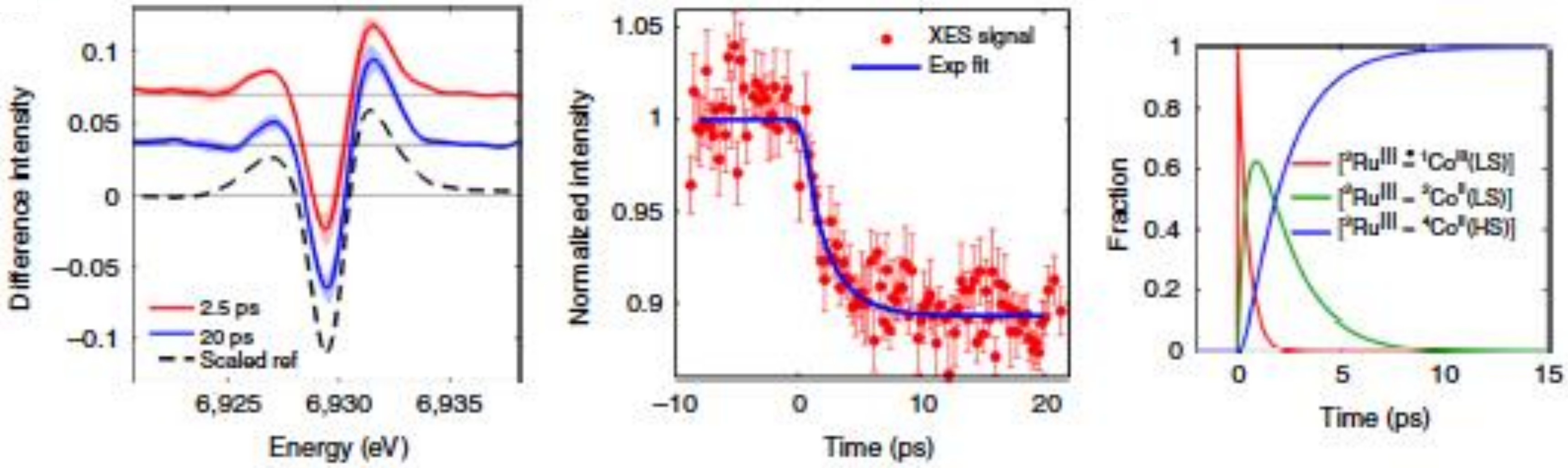
Combining X-ray spectroscopy and scattering (< 1 ps)





S. Canton *et al.*,

Nature Communications (2015)



Examples for chemical dynamics

LETTER

doi:10.1038/nature14163

...tion

...[1,2], Hosung Ki[1,2],
...ke Tono[5],
...ichi Adachi[3,8]

Selected for a Viewpoint in *Physics*

PRL 114, 255501 (2015) PHYSICAL REVIEW LETTERS week ending 26 JUNE 2015

...cond X-Ray Scattering
...cal Reaction

...son,[1] D. Ratner,[1] T. J. Lane,[1,4] D. Zhu,[1]
... Feng,[1] S. Nelson,[1] K. Saita,[3] B. Stankus,[2]
...l P. M. Weber[2,‡]

Probing the transition state region in catalytic CO oxidation on Ru

...Gladh,[1]
...chmann,[4]
...Minitti,[7]
...n,[11]

ARTICLE

Received 7 Oct 2014 | Accepted 23 Jan 2015 | Published 2 Mar 2015 DOI: 10.1038/ncomms7359 OPEN

Visualizing the non-equilibrium dynamics of photoinduced intramolecular electron transfer with femtosecond X-ray pulses

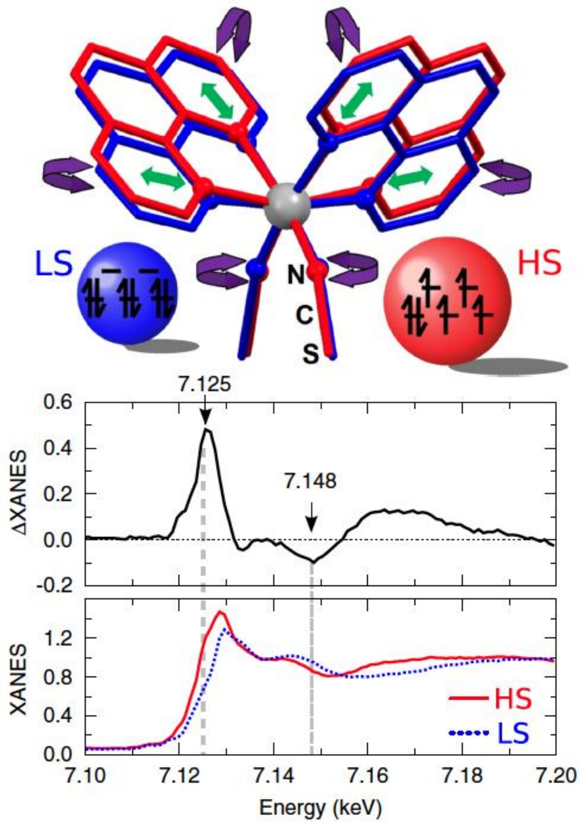
Sophie E. Canton[1,*], Kasper S. Kjær[2,3,*], György Vankó[4], Tim B. van Driel[3], Shin-ichi Adachi[5], Amélie Bordage[4,†], Christian Bressler[6,7], Pavel Chabera[8], Morten Christensen[3], Asmus O. Dohn[9], Andreas Galler[6], Wojciech Gawelda[6], David Gosztola[10], Kristoffer Haldrup[3], Tobias Harlang[8], Yizhu Liu[11], Klaus B. Møller[9], Zoltán Németh[4], Shunsuke Nozawa[5], Mátyás Pápai[4], Tokushi Sato[5,†], Takahiro Sato[12,†], Karina Suarez-Alcantara[1,†], Tadashi Togashi[13], Kensuke Tono[13], Jens Uhlig[8], Dimali A. Vithanage[8], Kenneth Wärnmark[11], Makina Yabashi[12], Jianxin Zhang[11,†], Villy Sundström[8] & Martin M. Nielsen[3]

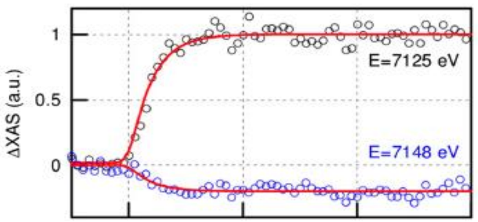
Some early experiments using XAS at XFELs

PRL 113, 227402 (2014) PHYSICAL REVIEW LETTERS week ending 28 NOVEMBER 2014

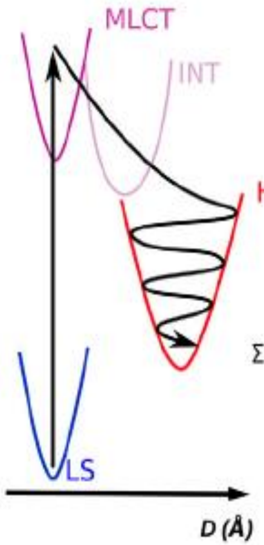
Sequential Activation of Molecular Breathing and Bending during Spin-Crossover Photoswitching Revealed by Femtosecond Optical and X-Ray Absorption Spectroscopy

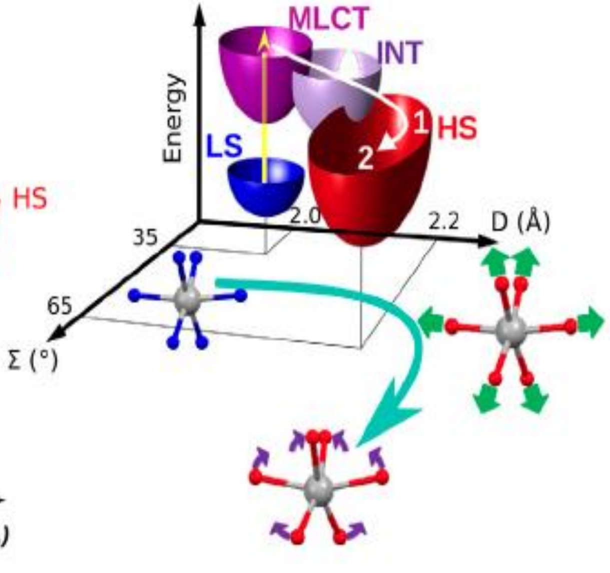
Marco Cammarata,[1] Roman Bertoni,[1] Maciej Lorenc,[1] Hervé Cailleau,[1] Sergio Di Matteo,[1] Cindy Mauriac,[2] Samir F. Matar,[2] Henrik Lemke,[3] Matthieu Chollet,[3] Sylvain Ravy,[4] Claire Laulhé,[4] Jean-François Létard,[2] and Eric Collet[1,*]





Ultrafast dynamics in molecular crystals during a photoinduced spin crossover has been characterized using the femtosecond X-ray absorption spectroscopy





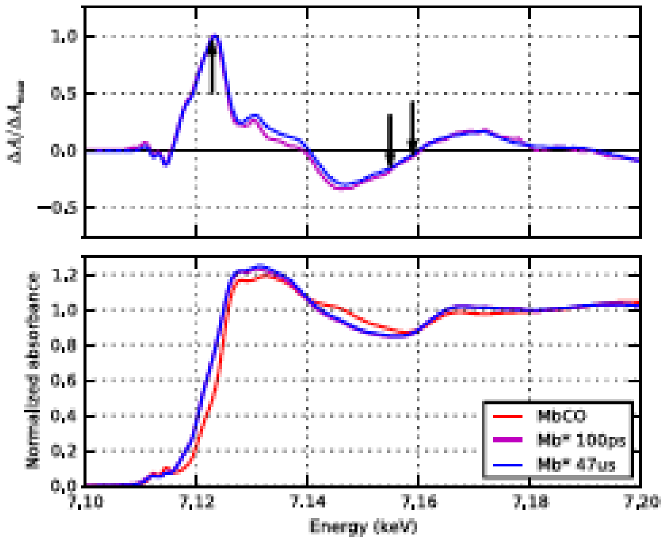
Ultrafast studies of CO detachment in MbCO

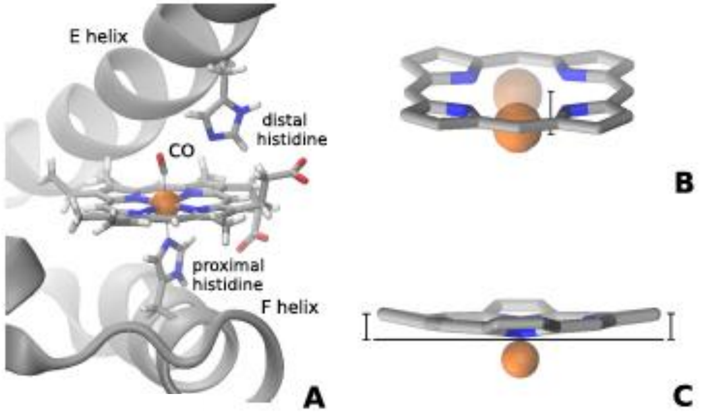
STRUCTURAL DYNAMICS 2, 041713 (2015)

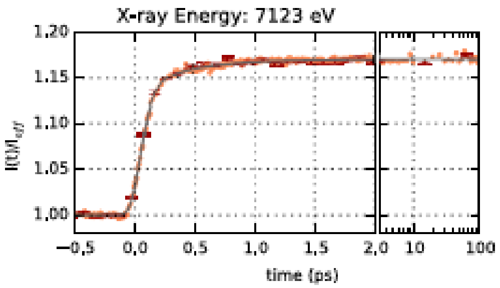
Observing heme doming in myoglobin with femtosecond X-ray absorption spectroscopy[a)]

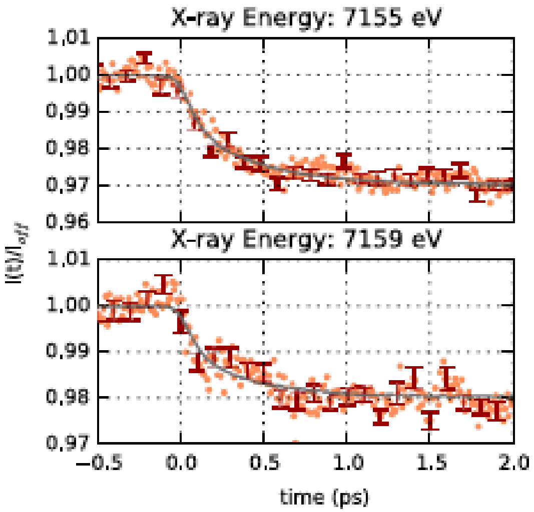
M. Levantino,[1] H. T. Lemke,[2] G. Schirò,[3] M. Glownia,[2] A. Cupane,[1] and M. Cammarata[4,b)]
[1]*Department of Physics and Chemistry, University of Palermo, Viale delle Scienze, 90128 Palermo, Italy*
[2]*LCLS, SLAC National Accelerator Laboratory, Menlo Park, California 94025, USA*
[3]*CNRS - Institut de Biologie Structurale, Grenoble 38044, France*
[4]*Department of Physics, UMR UR1-CNRS 6251, University of Rennes 1, Rennes, France*

(Received 5 March 2015; accepted 20 May 2015; published online 29 May 2015)









The XAS spectra of MbCO and decarboxymyoglobin have distinct spectral features in the XANES region. The ultrafast changes at selected resonances were probed with femtosecond time resolution

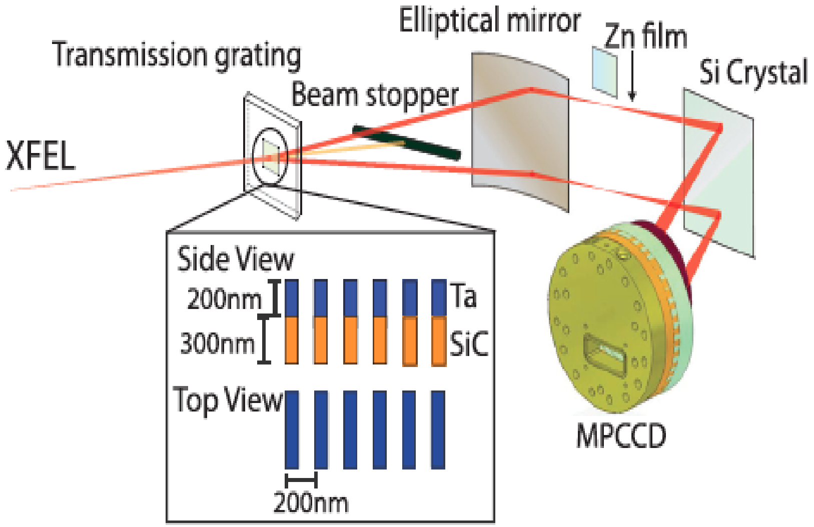
Alternative approaches to XAS at XFELs

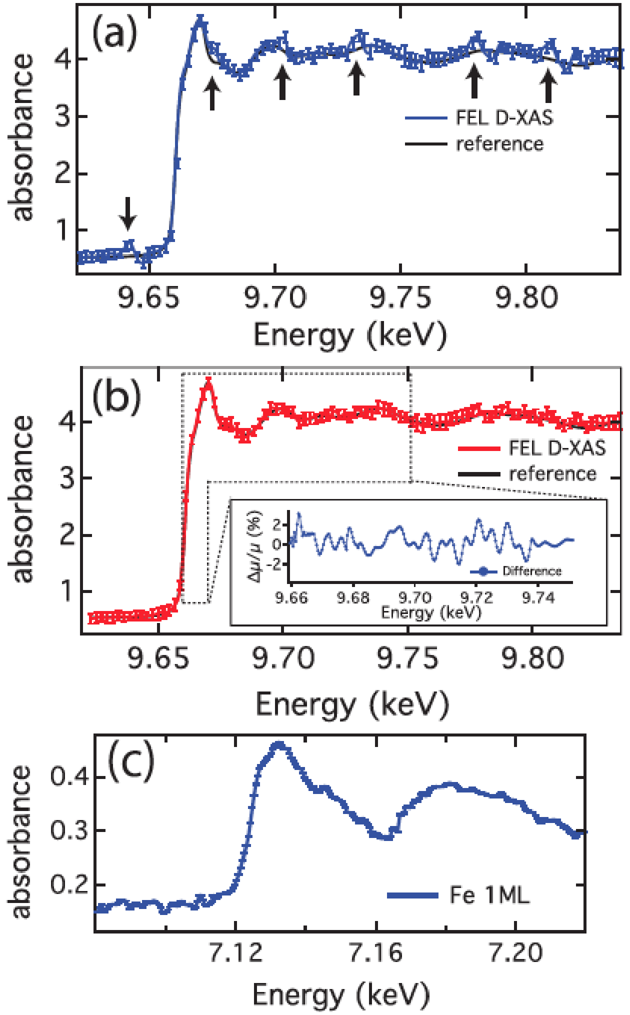
APPLIED PHYSICS LETTERS **103**, 131105 (2013)

Femtosecond x-ray absorption spectroscopy with hard x-ray free electron laser

Tetsuo Katayama,[1] Yuichi Inubushi,[2] Yuki Obara,[3] Takahiro Sato,[2,a)] Tadashi Togashi,[1] Kensuke Tono,[1] Takaki Hatsui,[2] Takashi Kameshima,[1] Atanu Bhattacharya,[4,b)] Yoshihiro Ogi,[5] Naoya Kurahashi,[4] Kazuhiko Misawa,[3] Toshinori Suzuki,[4,5] and Makina Yabashi[2,c)]

Dispersive geometry allows to mitigate the noisy nature of SASE XFELs and "self-normalize" the spectrum shot-by-shot.
However, the sensitivity is still limited to highly concentrated samples and poses very strict requirements on the X-ray optics

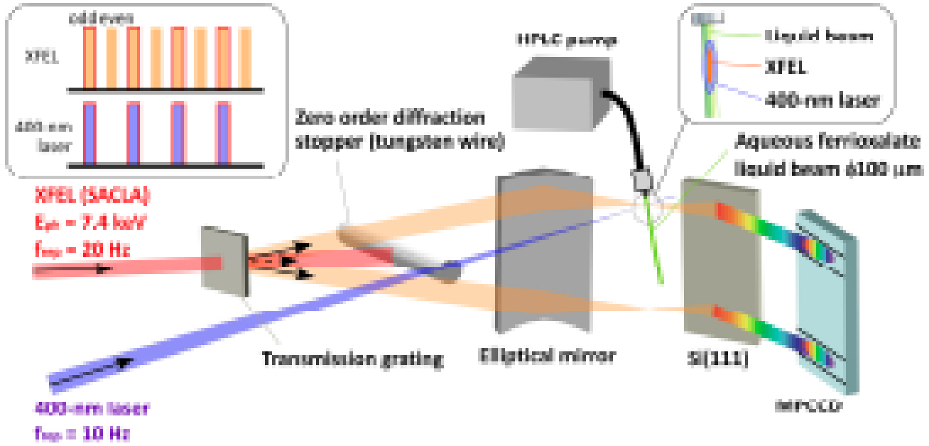


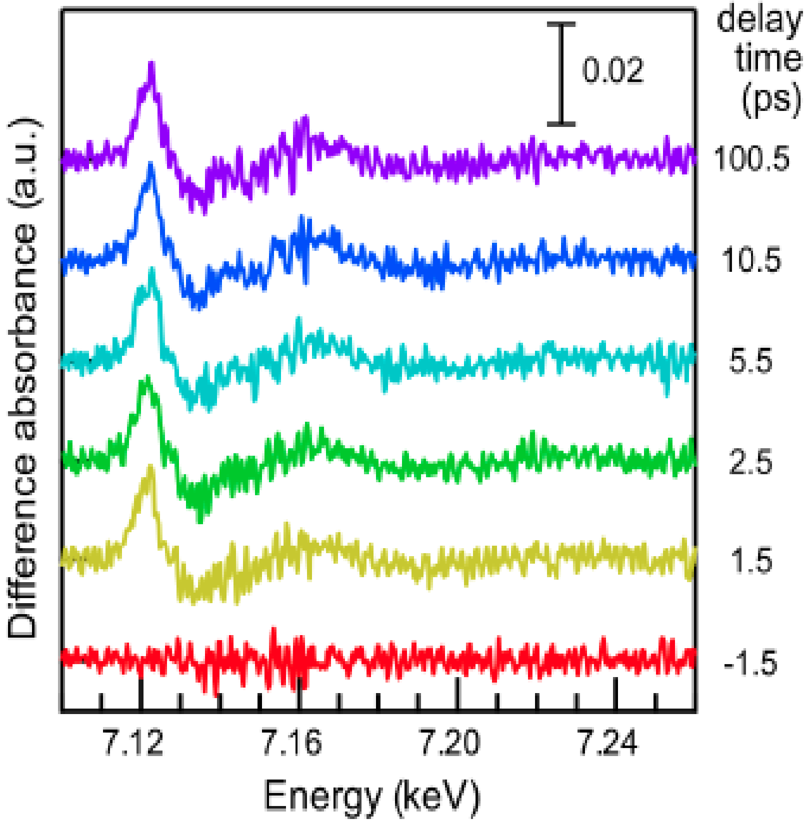


First example of time-resolved dispersive XAS

Femtosecond time-resolved X-ray absorption spectroscopy of liquid using a hard X-ray free electron laser in a dual-beam dispersive detection method

Yuki Obara,[1] Tetsuo Katayama,[2] Yoshihiro Ogi,[3] Takayuki Suzuki,[1,4] Naoya Kurahashi,[5] Shutaro Karashima,[5] Yuhei Chiba,[1] Yusuke Isokawa,[1] Tadashi Togashi,[6] Yuichi Inubushi,[6] Makina Yabashi,[6] Toshinori Suzuki,[3,5] and Kazuhiko Misawa[1,4,*]





Y. Obara *et al.*,
Optics Express, **22** (2014) 1105

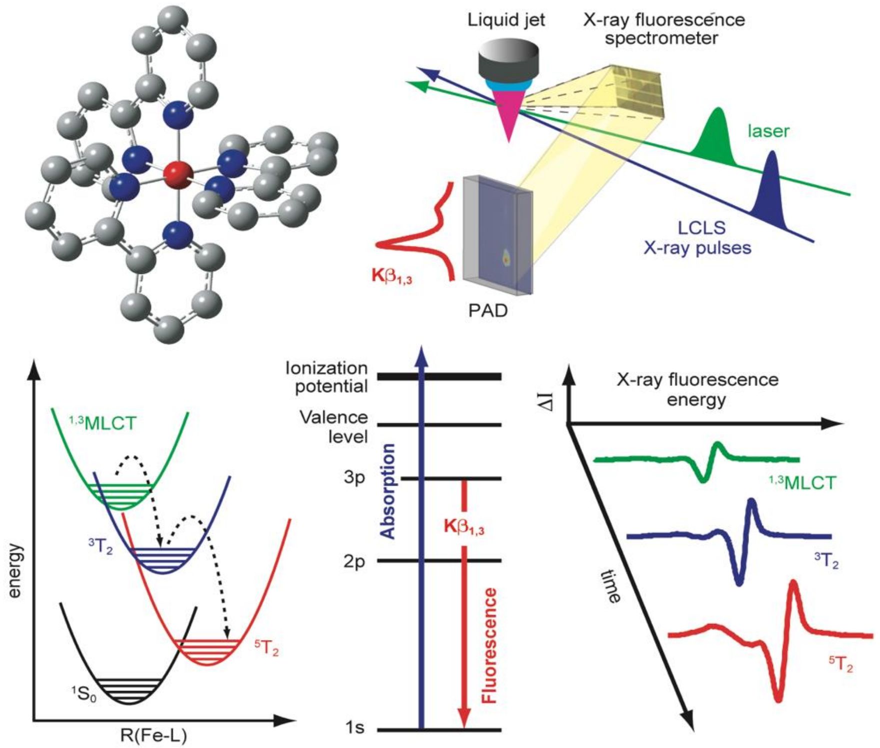
Femtosecond X-ray Emission Spectroscopy reveals "hidden" excited states

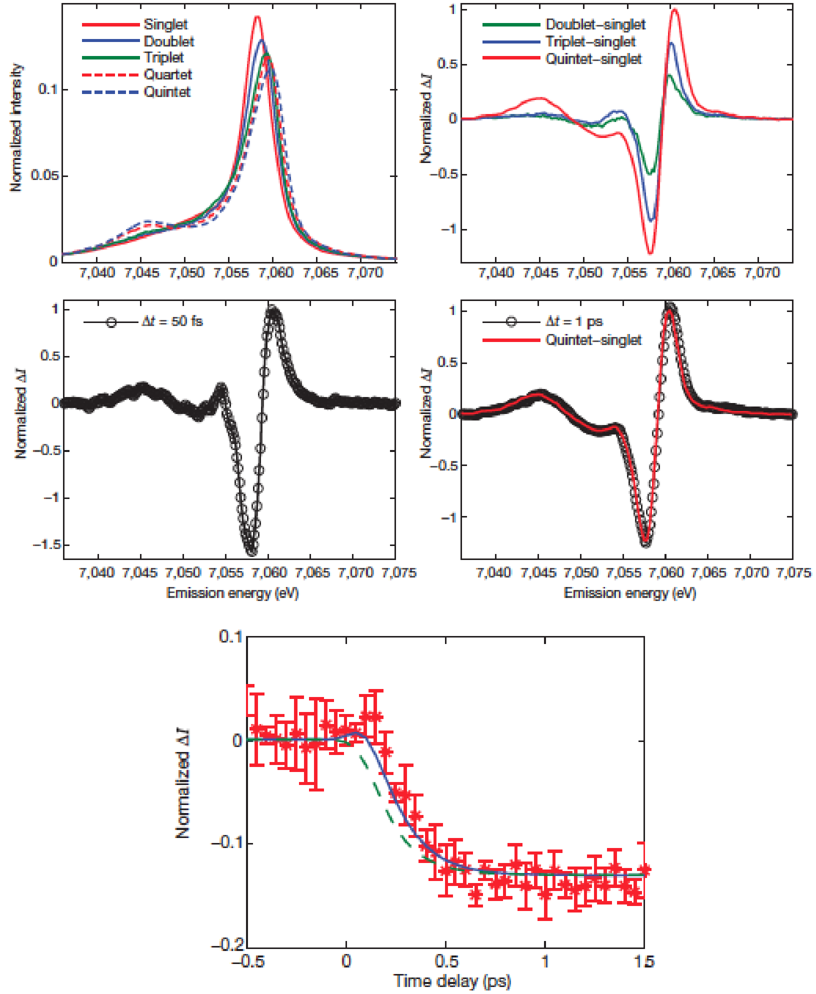
LETTER

doi:10.1038/nature13252

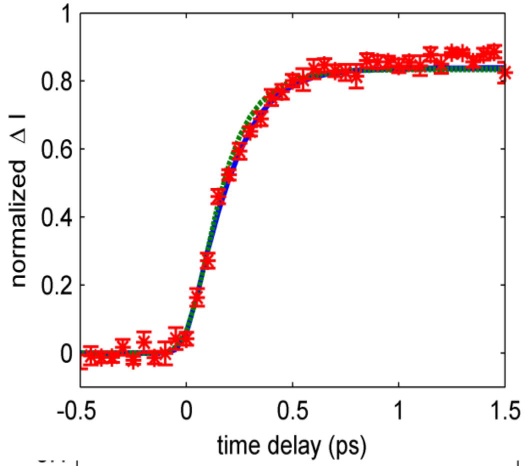
Tracking excited-state charge and spin dynamics in iron coordination complexes

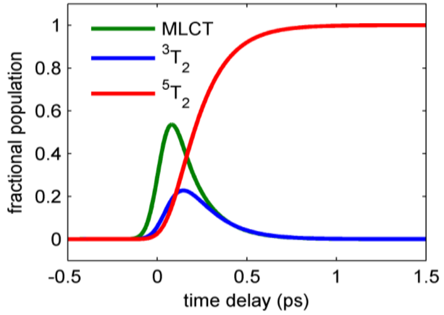
Wenkai Zhang[1], Roberto Alonso-Mori[2], Uwe Bergmann[2], Christian Bressler[3], Matthieu Chollet[2], Andreas Galler[3], Wojciech Gawelda[3], Ryan G. Hadt[4], Robert W. Hartsock[1,4], Thomas Kroll[4], Kasper S. Kjær[5,6], Katharina Kubiček[7,8], Henrik T. Lemke[2], Huiyang W. Liang[1,4], Drew A. Meyer[1,4], Martin M. Nielsen[6], Carola Purser[1], Joseph S. Robinson[2], Edward I. Solomon[4,9], Zheng Sun[1], Dimosthenis Sokaras[9], Tim B. van Driel[6], György Vankó[10], Tsu-Chien Weng[9], Diling Zhu[2] & Kelly J. Gaffney[1]

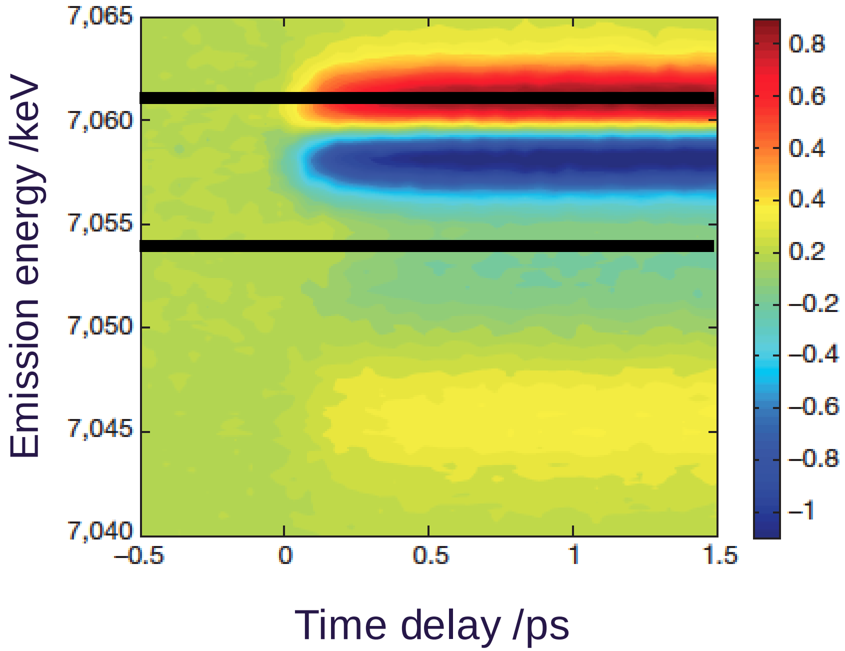


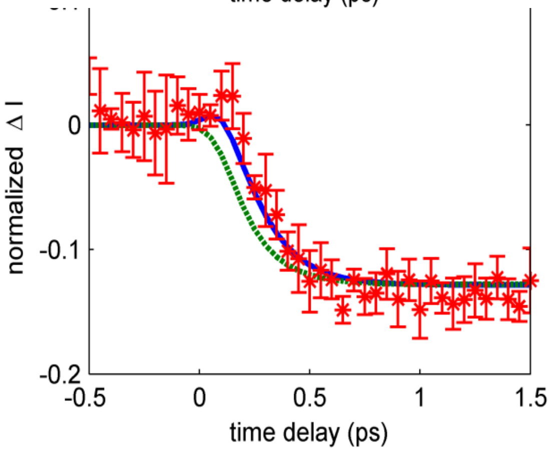


Femtosecond X-ray Emission Spectroscopy reveals "hidden" excited states









2D plot of time-dependent difference Kβ emission shows all photoinduced changes at very early time delays (< 2ps)

Kinetic model	lifetime	lifetime	Time zero	Instrument response	
	$1/k_1$(fs)	$1/k_2$(fs)	t_0(fs)	σ(fs)	FWHM(fs)
with triplet transient	150±50	70±30	0±7	56±8	130±20
without triplet transient	140±12		15±6	70±7	170±15

W. Zhang *et al.*, Nature, **509** (2014) 345

Observation of fs bond formation

Probe several time scales using FEL and SR sources

Use amorphous scattering to probe Au-Au bonds

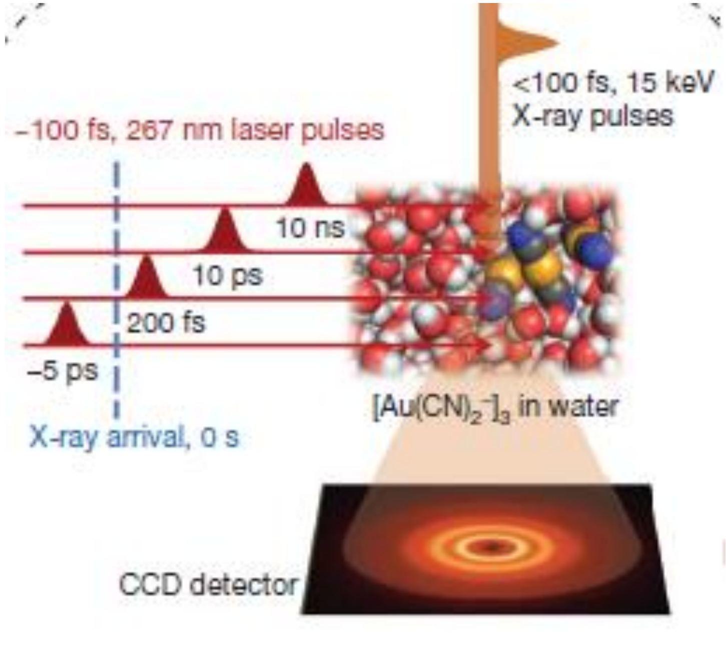
LETTER

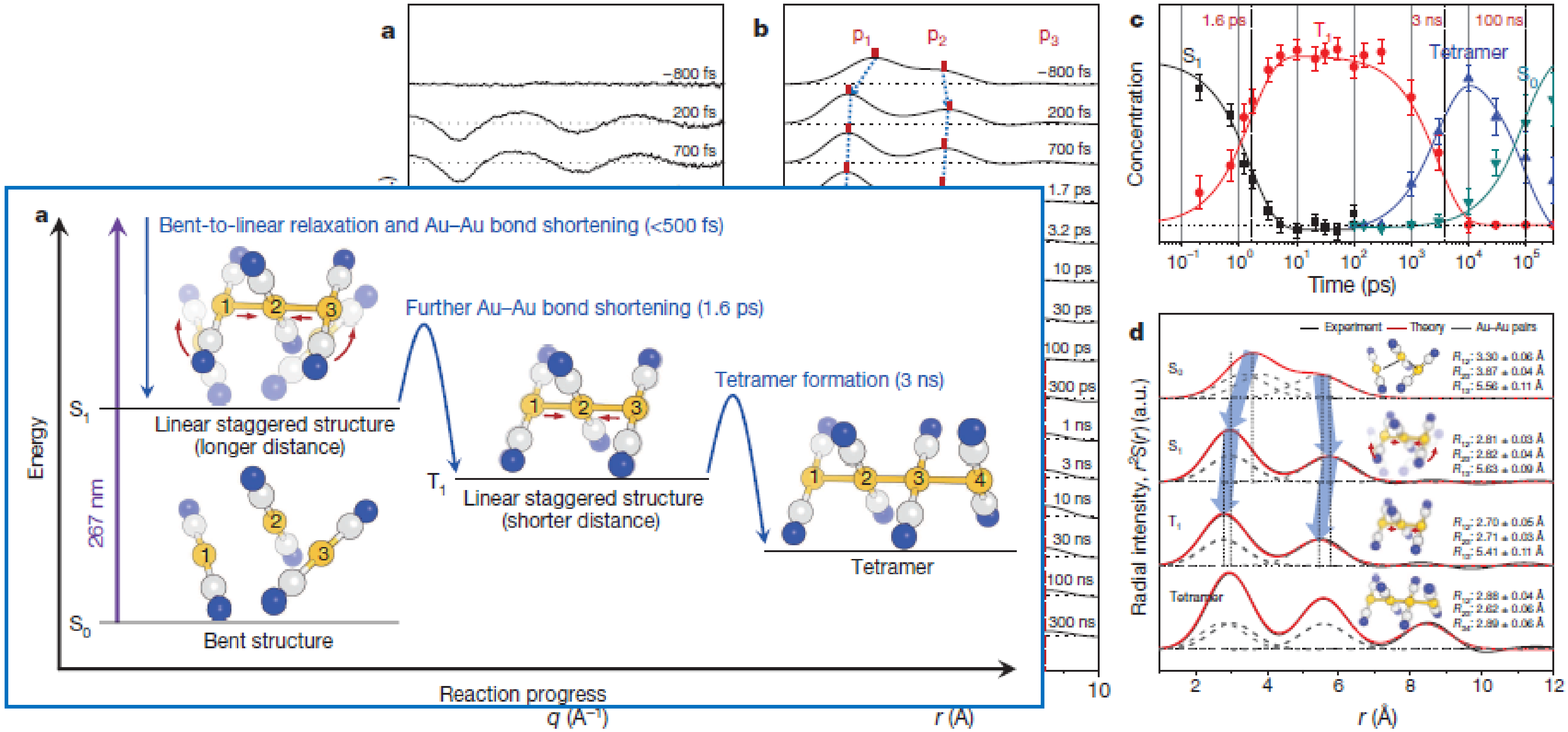
doi:10.1038/nature14163

Direct observation of bond formation in solution with femtosecond X-ray scattering

Kyung Hwan Kim[1,2]*, Jong Goo Kim[1,2]*, Shunsuke Nozawa[3]*, Tokushi Sato[3]†*, Key Young Oang[1,2], Tae Wu Kim[1,2], Hosung Ki[1,2], Junbeom Jo[1,2], Sungjun Park[1,2], Changyong Song[4], Takahiro Sato[4]†, Kanade Ogawa[4]†, Tadashi Togashi[5], Kensuke Tono[5], Makina Yabashi[4], Tetsuya Ishikawa[4], Joonghan Kim[6], Ryong Ryoo[1,2], Jeongho Kim[7], Hyotcherl Ihee[1,2] & Shin-ichi Adachi[3,8]

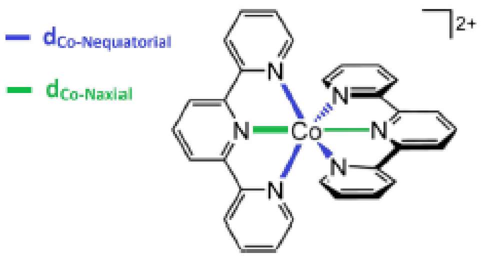
K.H. Kim et al., Nature 518, 790 (2015)

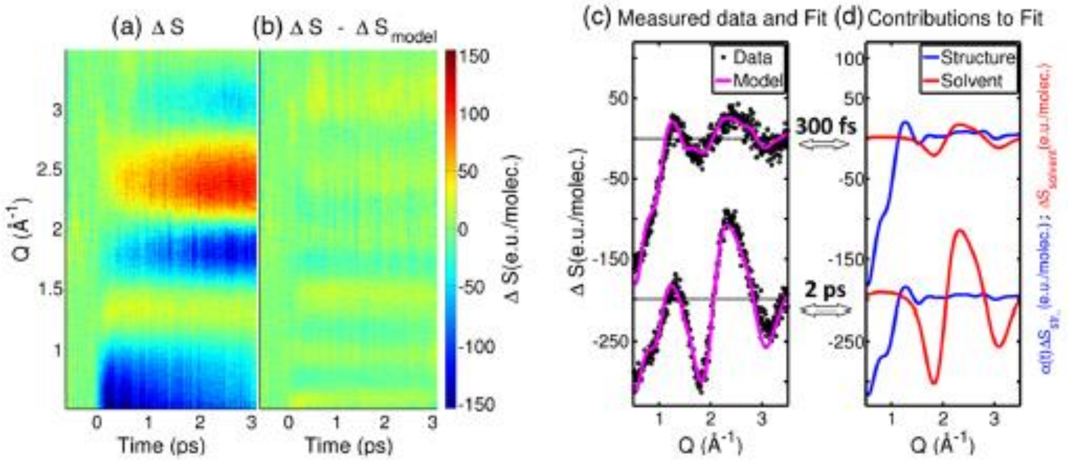




XFEL Science: new era in chemical reaction dynamics

Can we follow the coherent and incoherent dynamics?
Can we relate the vibrational coherence to molecular structure changes?





PRL 117, 013002 (2016) PHYSICAL REVIEW LETTERS week ending 1 JULY 2016

Femtosecond X-Ray Scattering Study of Ultrafast Photoinduced Structural Dynamics in Solvated $[Co(terpy)_2]^{2+}$

Elisa Biasin,[1] Tim Brandt van Driel,[1] Kasper S. Kjær,[1,2,3] Asmus O. Dohn,[4] Morten Christensen,[1] Tobias Harlang,[2] Pavel Chabera,[2] Yizhu Liu,[2,5] Jens Uhlig,[2] Mátyás Pápai,[4,6] Zoltán Németh,[6] Robert Hartsock,[3] Winnie Liang,[3] Jianxin Zhang,[7] Roberto Alonso-Mori,[8] Matthieu Chollet,[8] James M. Glownia,[8] Silke Nelson,[8] Dimosthenis Sokaras,[8] Tadesse A. Assefa,[9] Alexander Britz,[9] Andreas Galler,[9] Wojciech Gawelda,[9,10] Christian Bressler,[9] Kelly J. Gaffney,[3] Henrik T. Lemke,[8,11] Klaus B. Møller,[4] Martin M. Nielsen,[1] Villy Sundström,[2] György Vankó,[6] Kenneth Wärnmark,[5] Sophie E. Canton,[12,13] and Kristoffer Haldrup[1,*]

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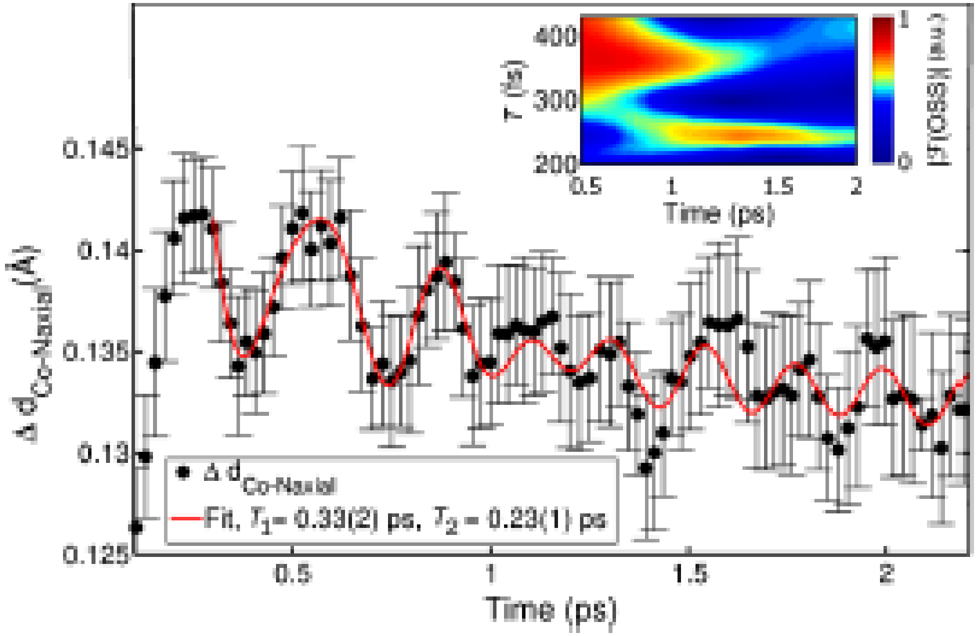
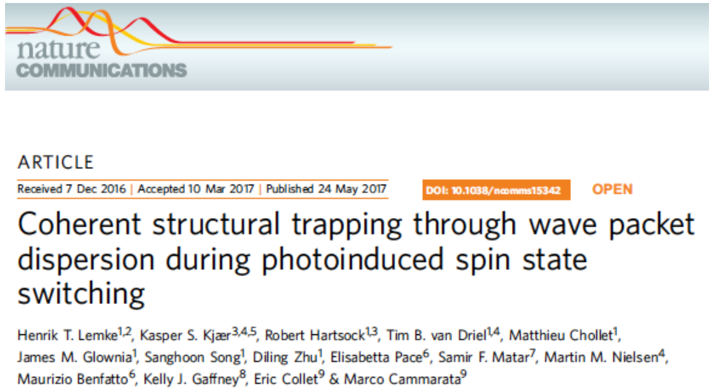
[12]*IFG Structural Dynamics of (Bio)chemical Systems, Max Planck Institute for Biophysical Chemistry, Am Fassberg 11, D-37077 Goettingen, Germany*
[13]*FS-SCS, Structural Dynamics with Ultra-short Pulsed X-rays, Deutsches Elektronen-Synchrotron (DESY), Notkestrasse 85, D-22607 Hamburg, Germany*

(Received 5 February 2016; published 30 June 2016)



XFEL allowed for the first time to observe coherent vibrational wavepackets in molecular systems in liquid phase!

Pioneering work on coherent wavepacket dynamics in solvated Fe(II) complex using femtosecond XAS

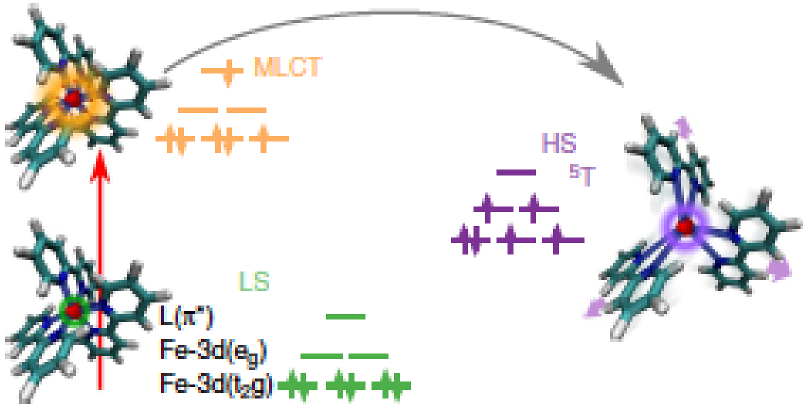

nature COMMUNICATIONS

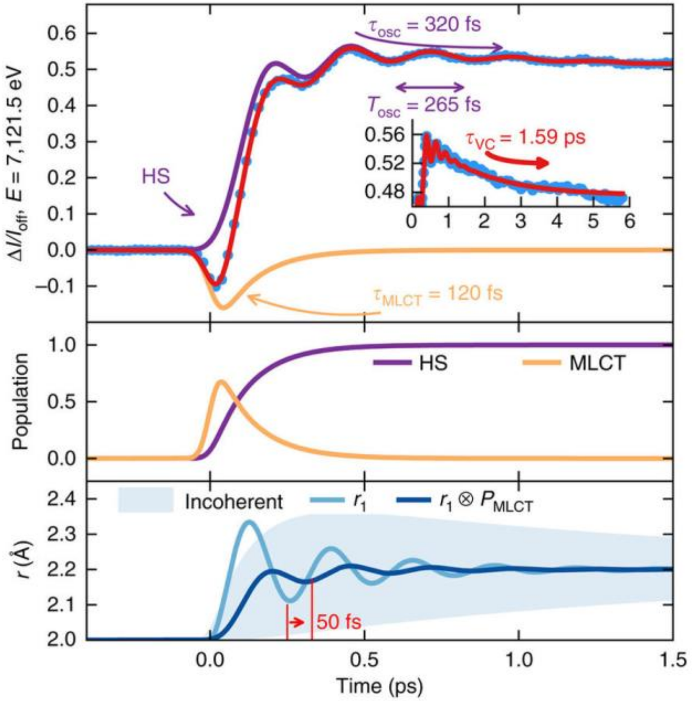
ARTICLE

Received 7 Dec 2016 | Accepted 10 Mar 2017 | Published 24 May 2017 DOI: 10.1038/ncomms15342 OPEN

Coherent structural trapping through wave packet dispersion during photoinduced spin state switching

Henrik T. Lemke[1,2], Kasper S. Kjær[3,4,5], Robert Hartsock[1,3], Tim B. van Driel[1,4], Matthieu Chollet[1], James M. Glownia[1], Sanghoon Song[1], Diling Zhu[1], Elisabetta Pace[6], Samir F. Matar[7], Martin M. Nielsen[4], Maurizio Benfatto[6], Kelly J. Gaffney[8], Eric Collet[9] & Marco Cammarata[9]

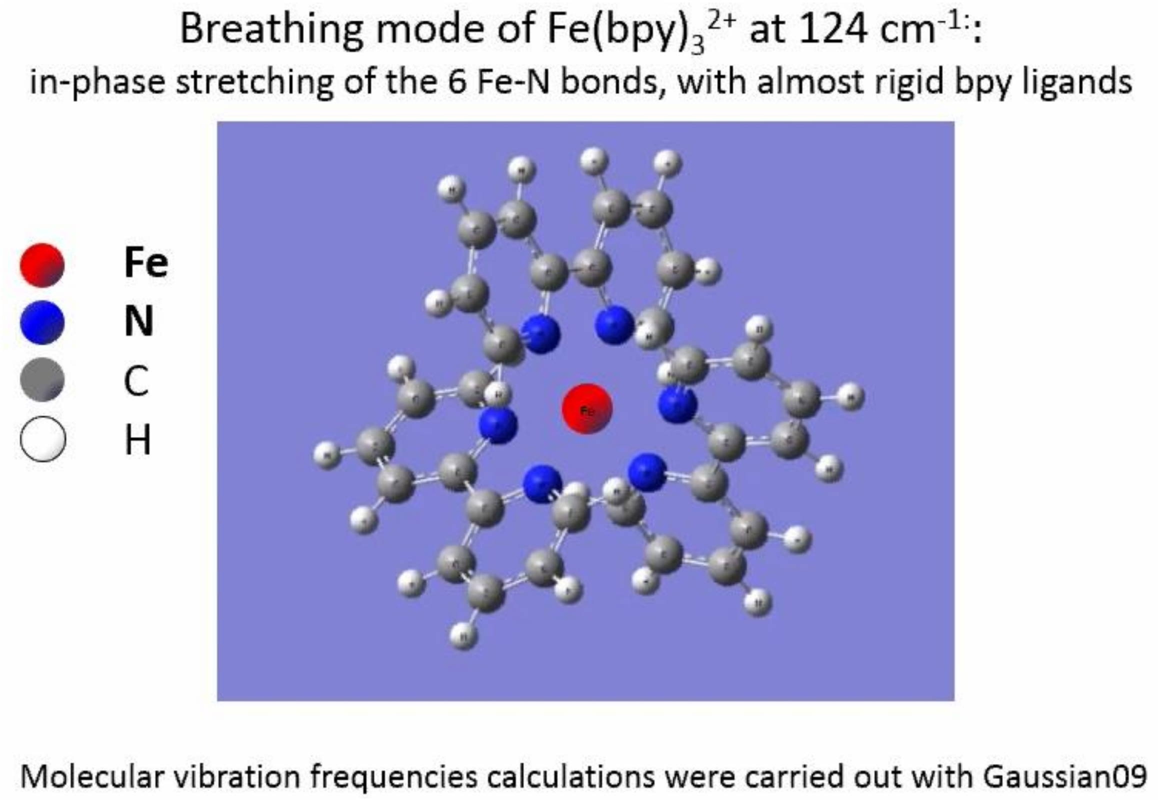


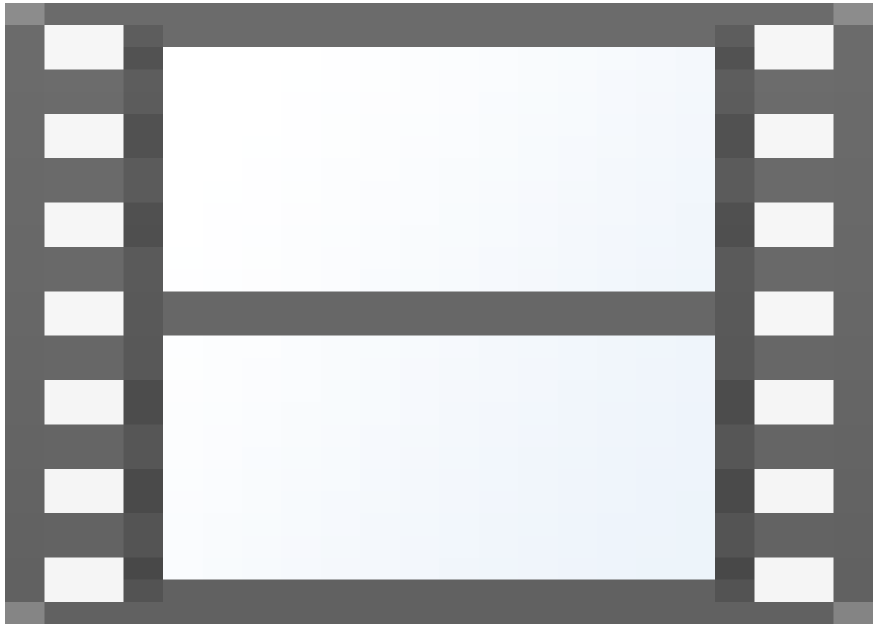


Very large structural changes due to a photoinduced spin transition
→ symmetric Fe-N bond elongation by 0.2 Å

H. Lemke, *et al.* Nat. Commun. 8 (2017) 15342

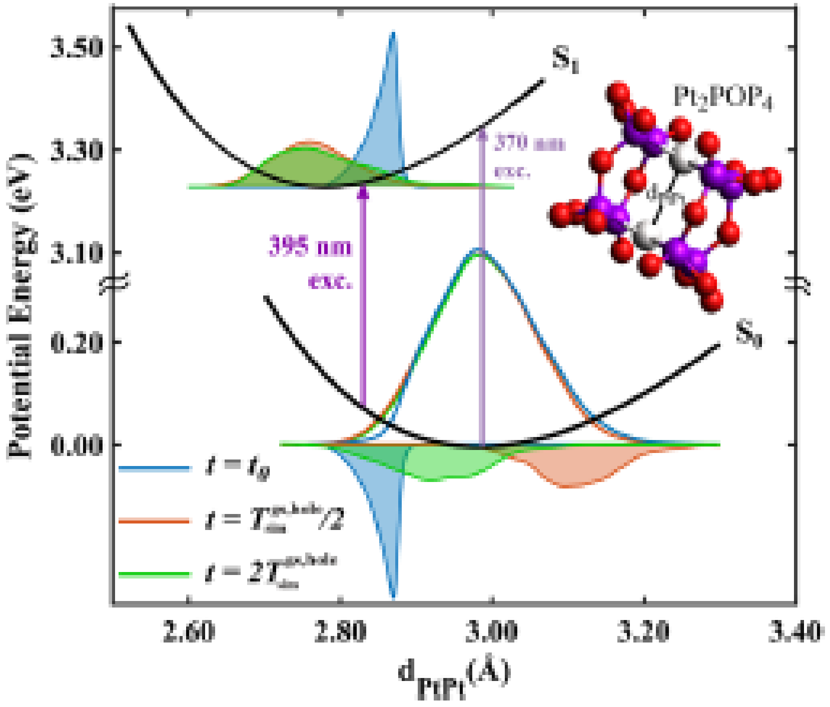
Real-time visualization of coherent atomic movements!





H. Lemke, *et al.* Nat. Commun. 8 (2017) 15342

Coherent nuclear dynamics captured with femtosecond X-rays



PHYSICAL REVIEW LETTERS **122,** 063001 (2019)

Editors' Suggestion

Ultrafast X-Ray Scattering Measurements of Coherent Structural Dynamics on the Ground-State Potential Energy Surface of a Diplatinum Molecule

Kristoffer Haldrup,[1] Gianluca Levi,[2,3] Elisa Biasin,[1,4] Peter Vester,[1] Mads Goldschmidt Laursen,[1] Frederik Beyer,[1] Kasper Skov Kjær,[1,5,4] Tim Brandt van Driel,[1,6] Tobias Harlang,[1,5] Asmus O. Dohn,[2,7] Robert J. Hartsock,[4] Silke Nelson,[6] James M. Glownia,[6] Henrik T. Lemke,[6,8] Morten Christensen,[1] Kelly J. Gaffney,[4] Niels E. Henriksen,[2] Klaus B. Møller,[2] and Martin M. Nielsen[1]

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[5]*Department of Chemical Physics, Lund University, Box 118, S-22100 Lund, Sweden*
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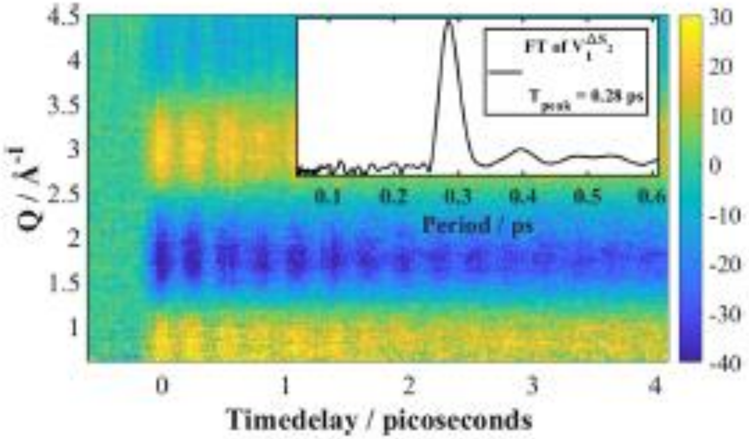
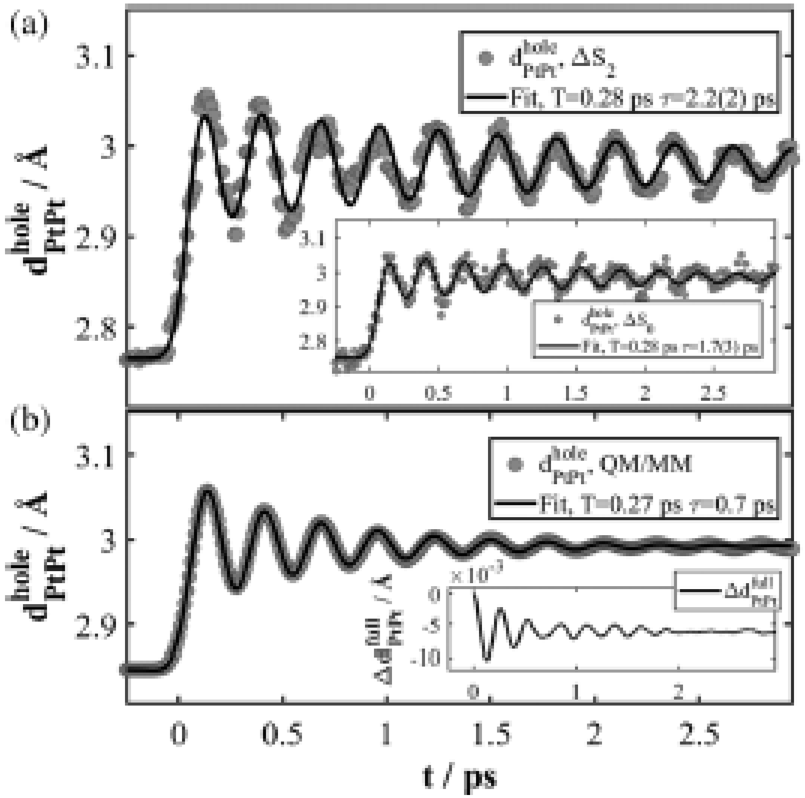
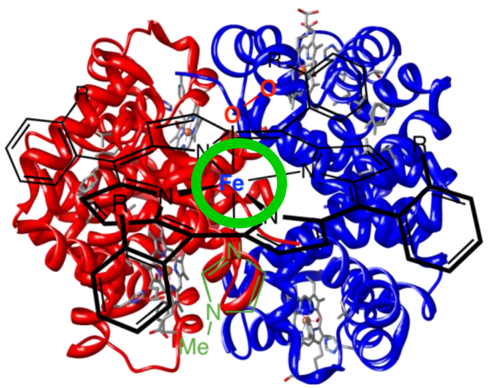
[8]*SwissFEL, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland*





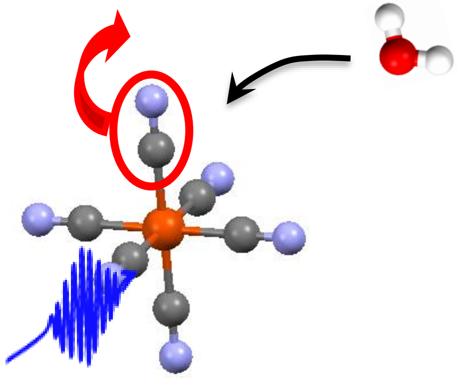
Ligand exchange in transition metal complexes

Oxygen transport: Hb

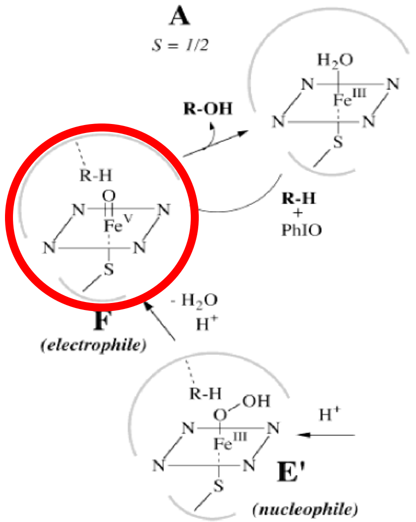


Iron(II) hexacyanide

in water



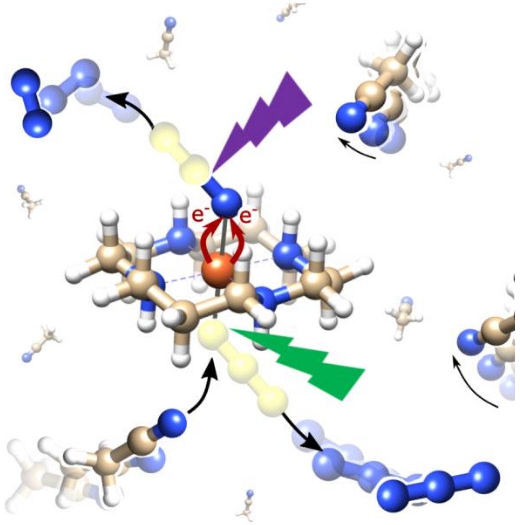
Drug metabolism: ***Cytochrome P450 superfamily of heme-enzymes***



B. Meunier, *et al.*, Chem. Rev. 104 (2004); J. Rittle and M. Green, Science 330 (2010)

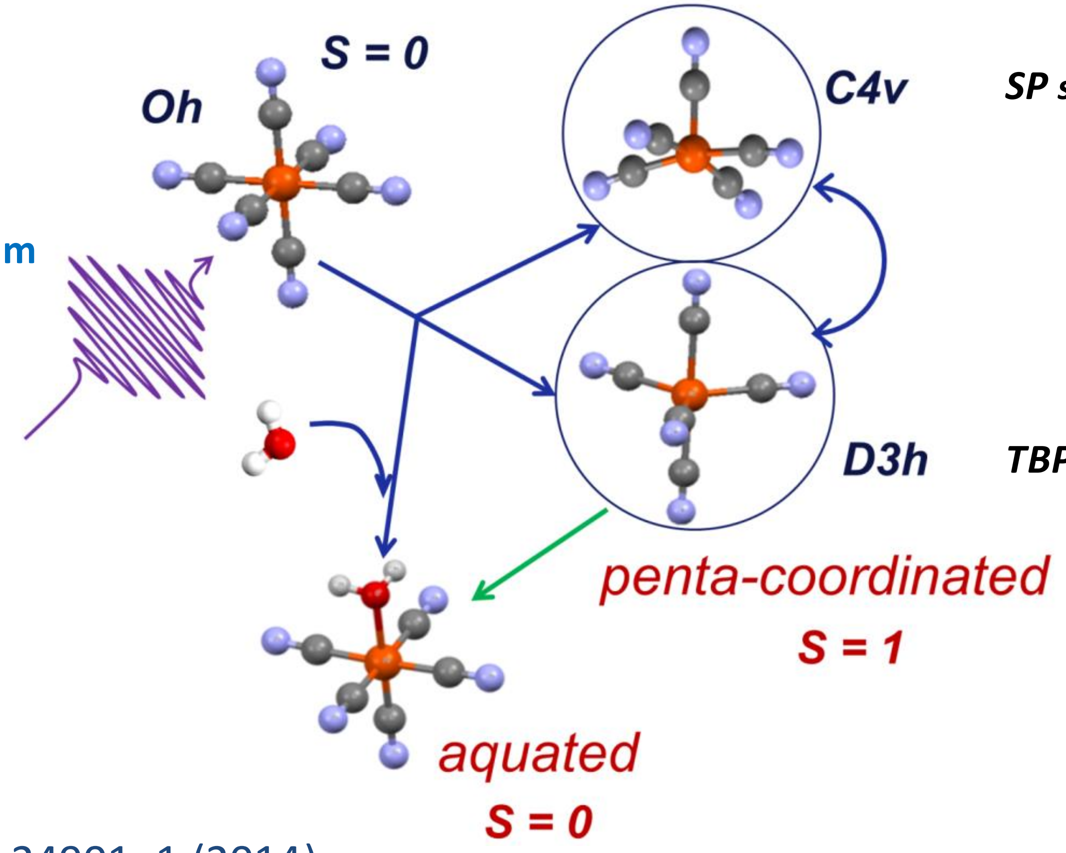
trans-[(cyclam)$Fe^{III}(N_3)_2$]$^+$

in acetonitrile



Structural dynamics in aqueous $Fe(CN)_6$

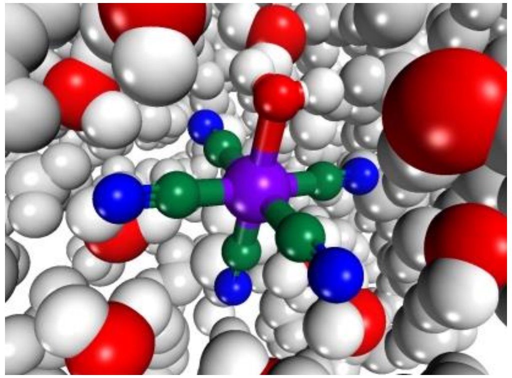
Iron(II) hexacyanide in H_2O



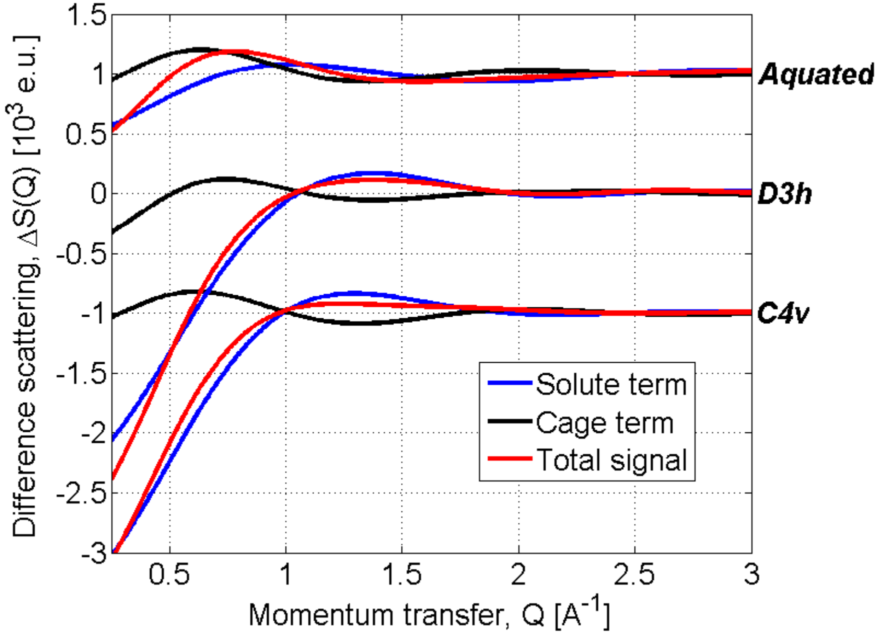
M. Reinhard et al., JACS (2017)

M. Reinhard et al., Struct. Dyn., 24901, 1 (2014)

Simulation of difference scattering for $Fe(CN)_6$

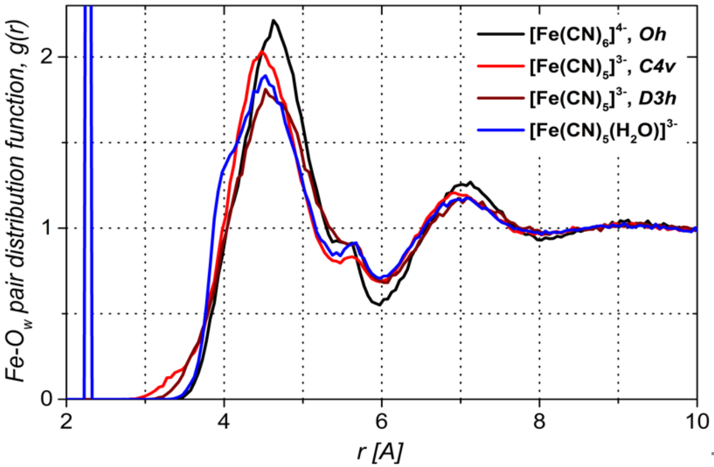


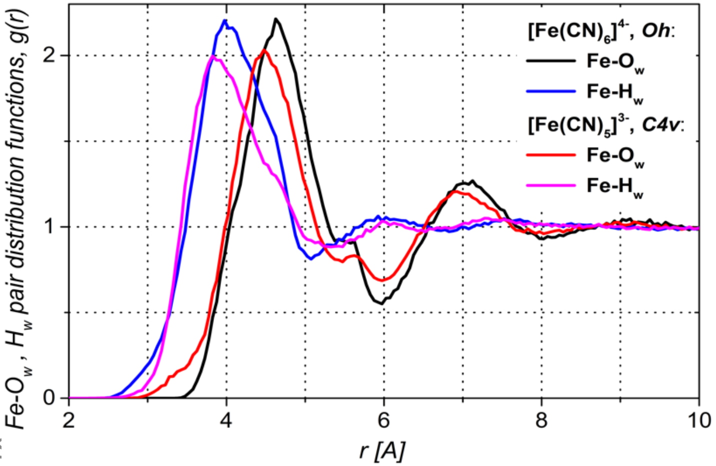
- Box size: 768 H_2O mol.
- TIP3P (flex.) water
- Simulation length: 5ns
- Canonical ensemble (NVT)
- Nosé-Hoover thermostat
- COMPASSII force field
- ESP charge partitioning for the solute
- Solute structure fixed



$$S_{solute}(Q) = \sum_n f_n^2(Q) + \sum_n \sum_{m \neq n} (f_n(Q) \cdot f_m(Q) \cdot \frac{sin(Q \cdot r_{nm})}{Q \cdot r_{nm}})$$

$$S_{cage}(Q) = \sum_n N_n f_n^2(Q) + \sum_n \sum_{m \neq n} (\frac{N_n N_m}{V} f_n(Q) \cdot f_m(Q) \int_0^\infty (g_{nm}(r) - 1) \cdot \frac{sin(Q \cdot r)}{Q \cdot r} \cdot 4\pi r^2 dr)$$



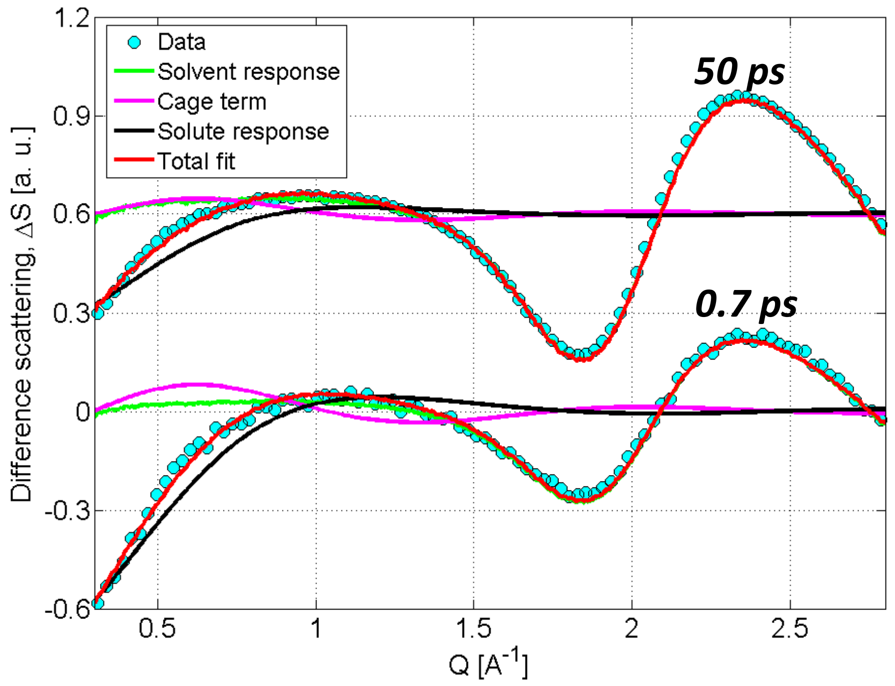


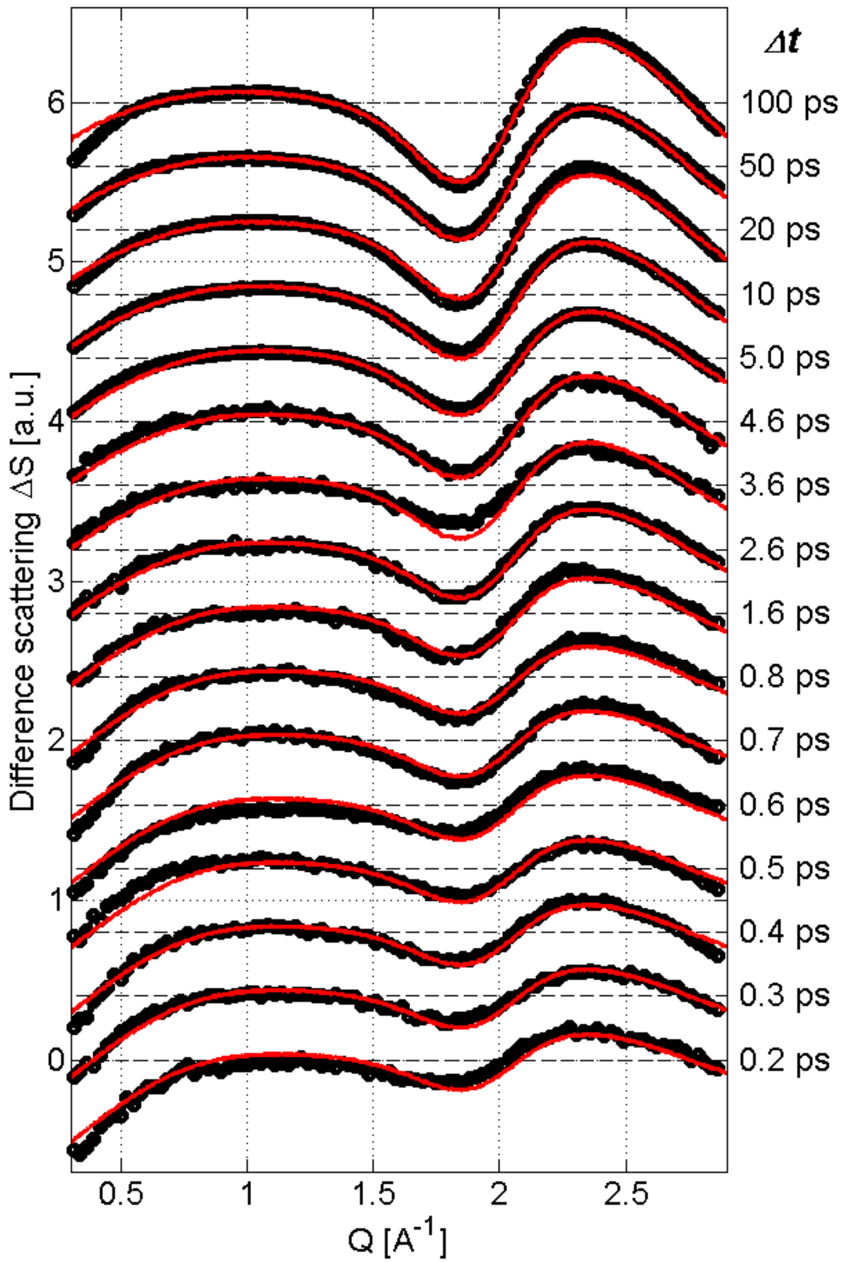
The local and the global kinetic fits

$$\Delta S_{sim}(Q,t) = \Delta S_{solute}(Q,t) + \Delta S_{cage}(Q,t) + \left(\frac{\partial S_{solv}(Q)}{\partial T}\cdot \Delta T(t)\right)$$

1) $Fe(CN)_5 + CN$ → $Fe(CN)_6$ *(ground state)*
2) $Fe(CN)_5$ → $Fe(CN)_5$ * *(separated fragment)*
3) $Fe(CN)_5 + H_2O$ → $Fe(CN)_5(H_2O)$ *(aquation*

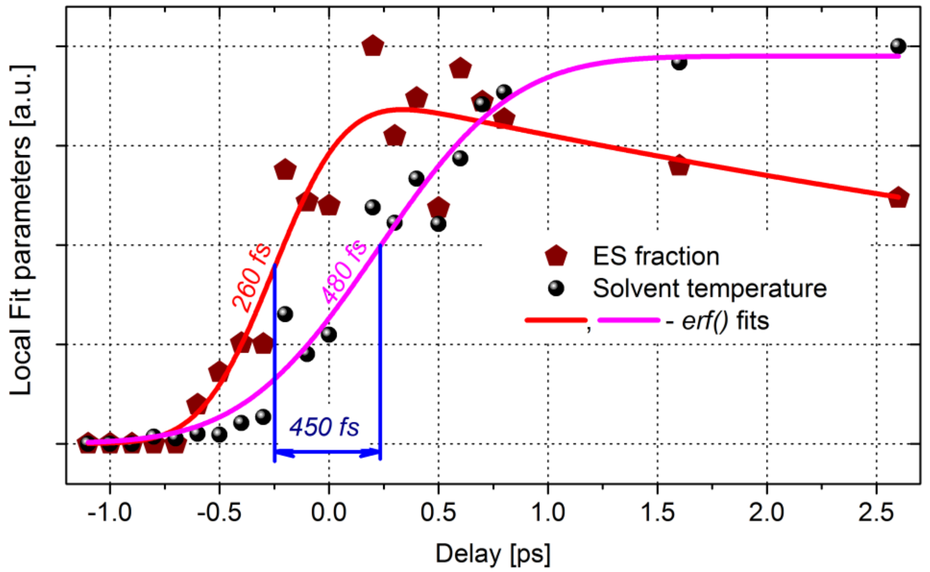
$\Delta T_{solv}(t) = (\sum c_k(t=0)E_{hv} - \sum c_k(t)E_k) / Cv$

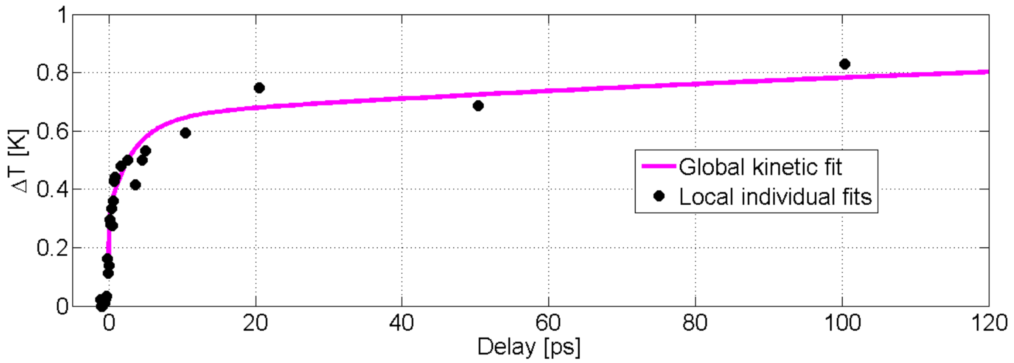


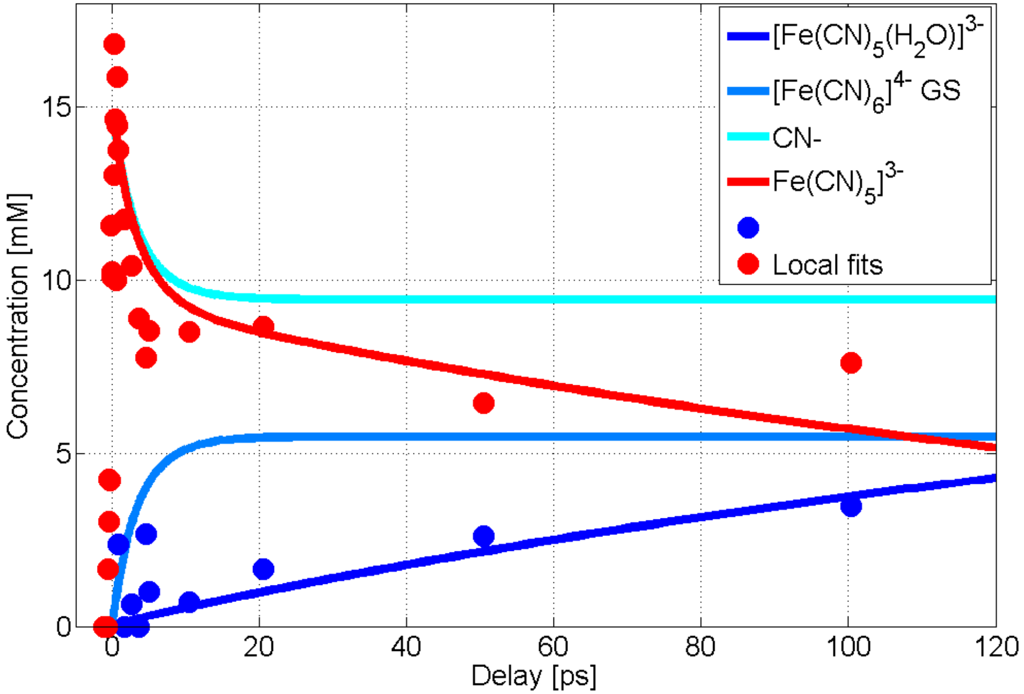


Species concentration and temperature kinetics

Delay in excess energy dissipation



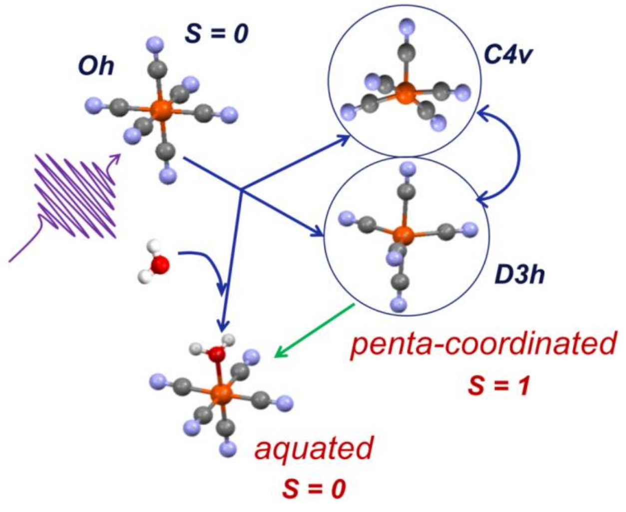




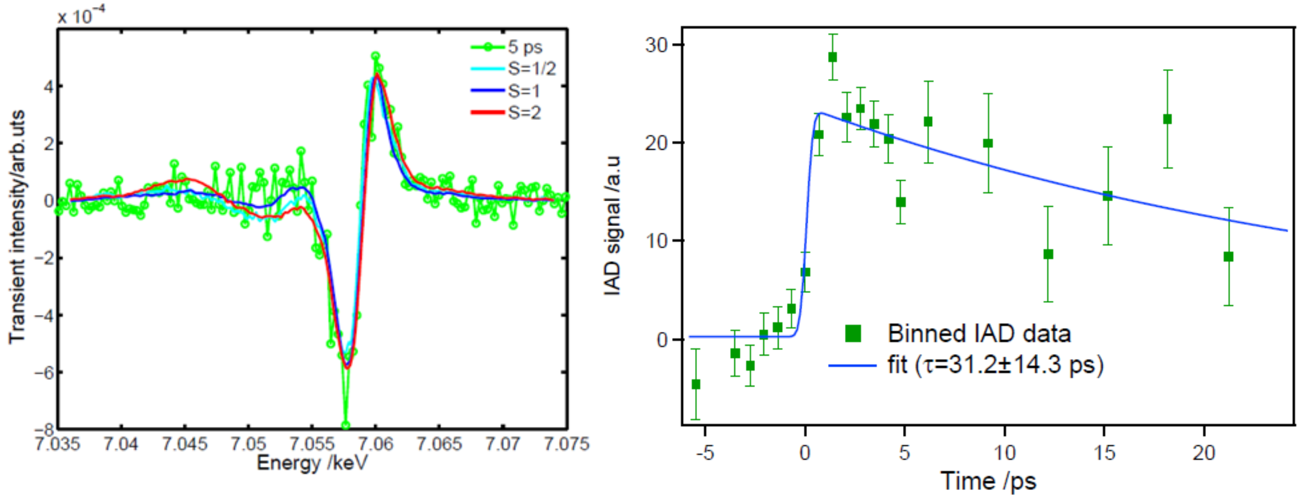
Non-geminate recombination $k_1 = 8 \times 10^{12}$ 1/(M*s) ~ 6 ps

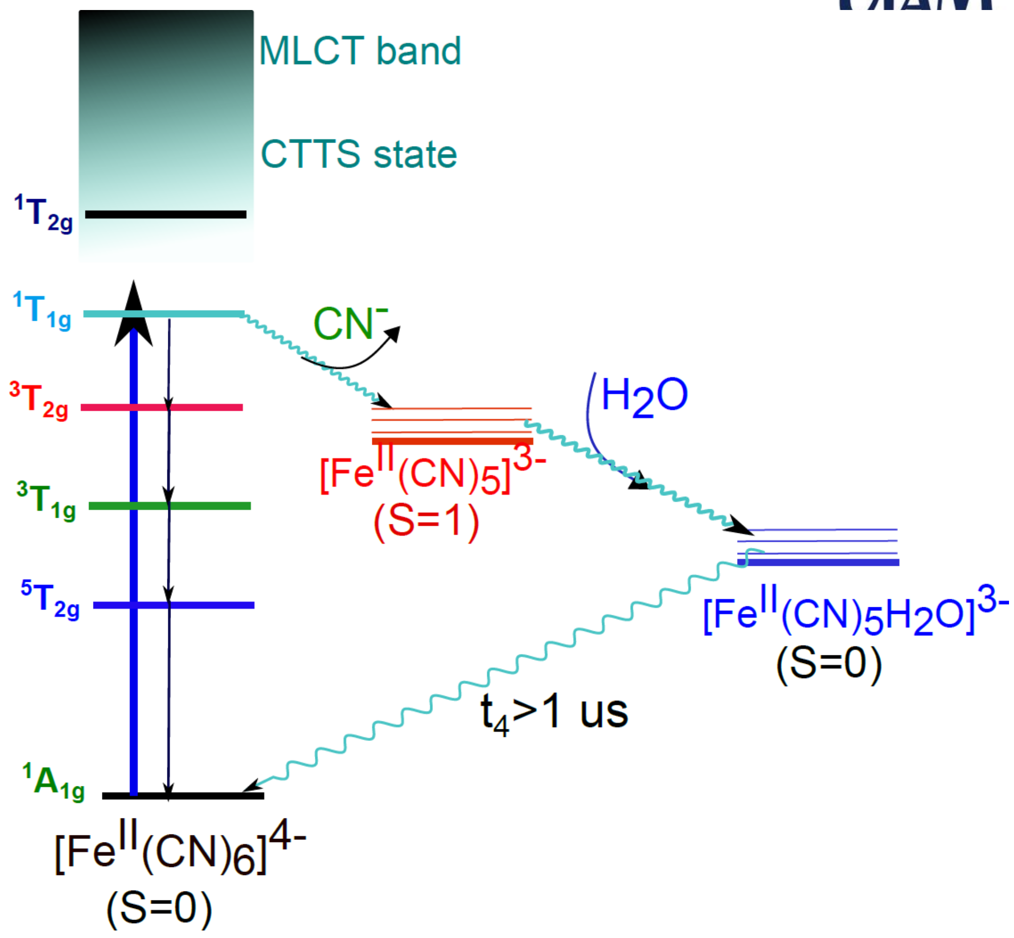
Aquation $k_3 = 9 \times 10^{7}$ 1/(M*s) ~ 100 ps

Spin state of the intermediate species



Difference Kb XES spectra – triplet multiplicity

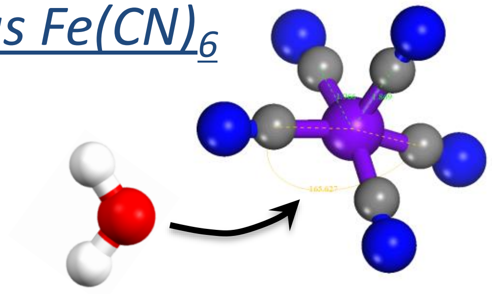


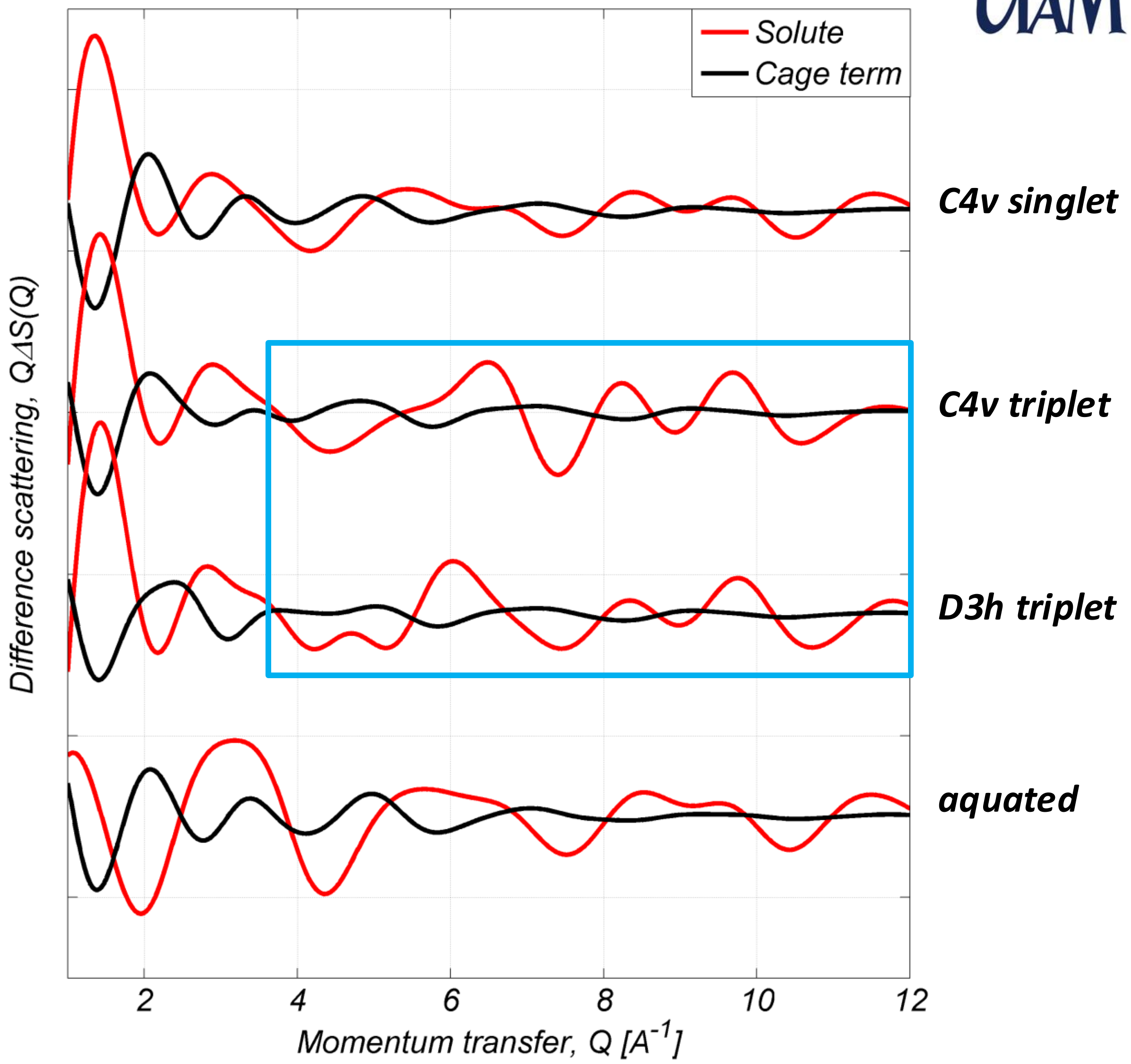


Courtesy by Tadesse Assefa

Perspective: high resolution X-ray scattering

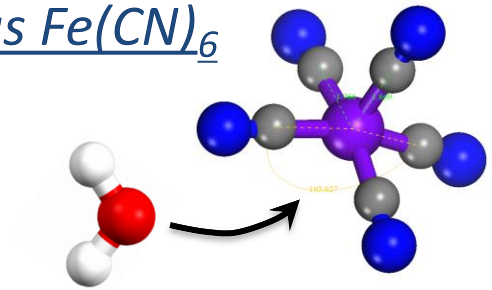
Aqueous $Fe(CN)_6$





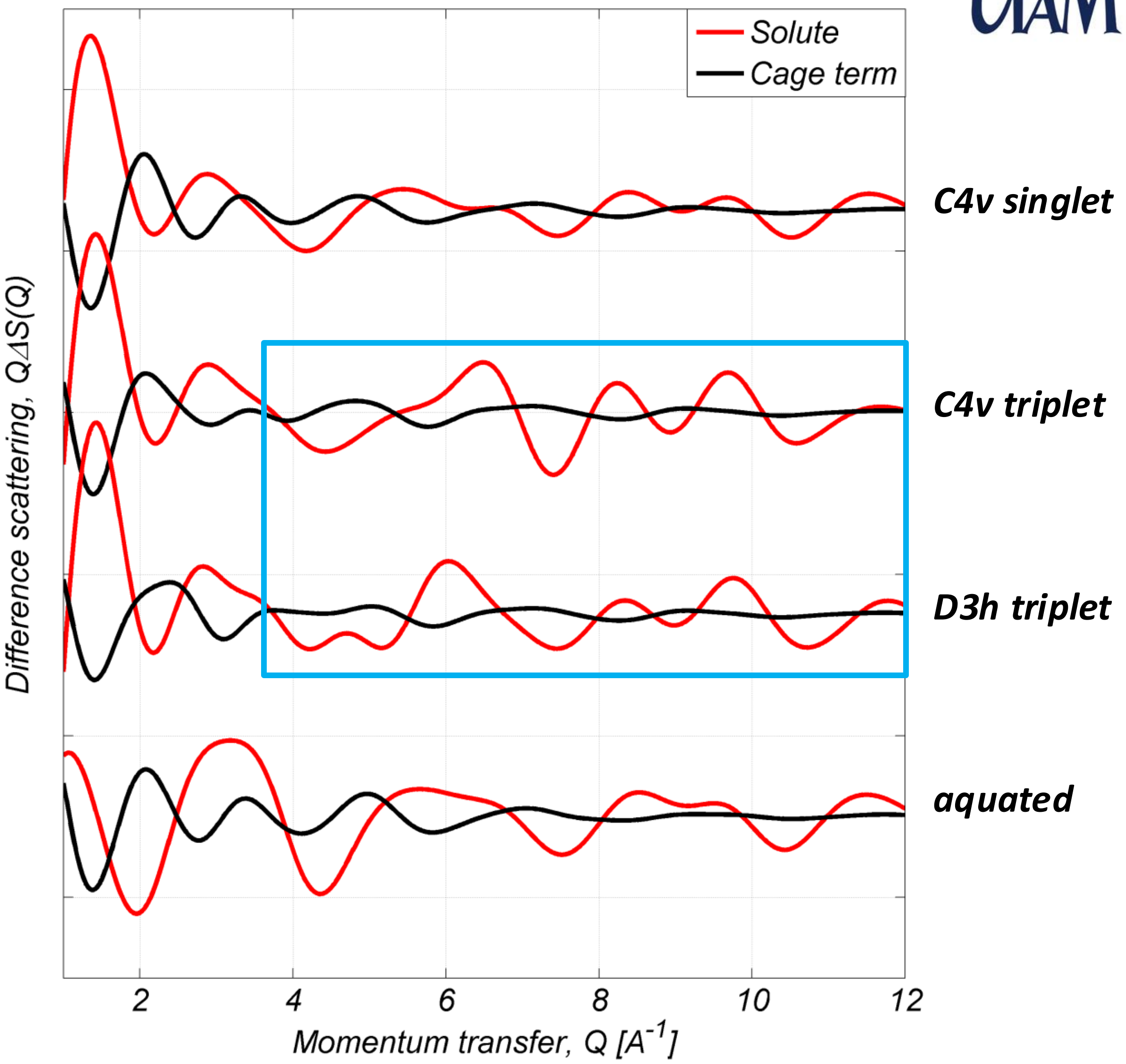
Perspective: high resolution X-ray scattering

Aqueous $Fe(CN)_6$



Large reciprocal space coverage:

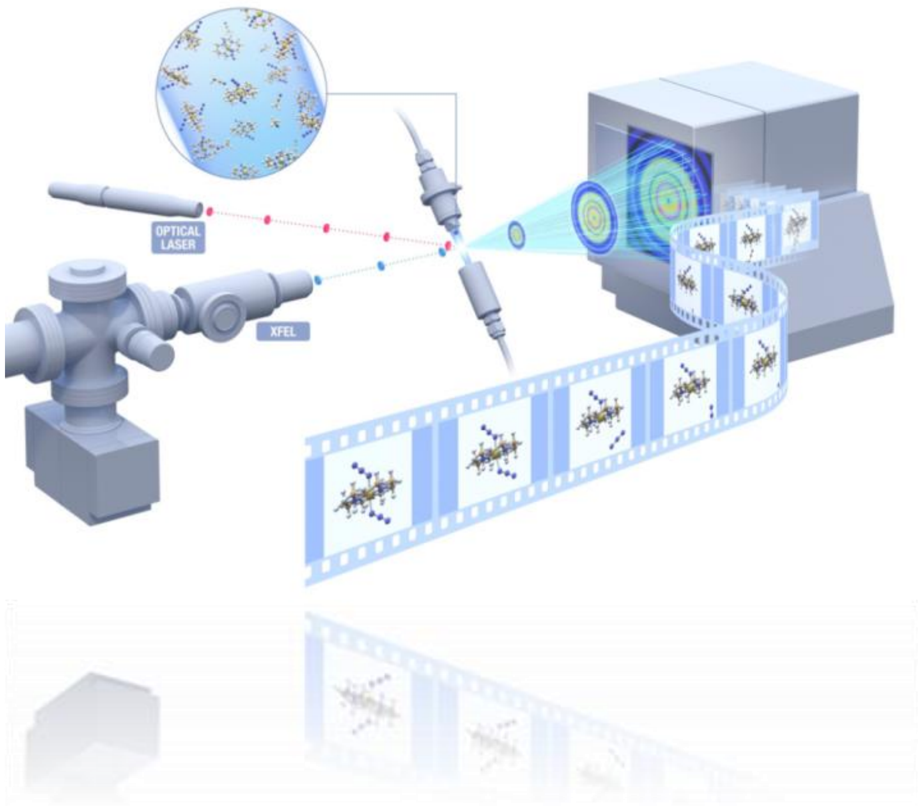
High X-ray energy and Large Area Detector

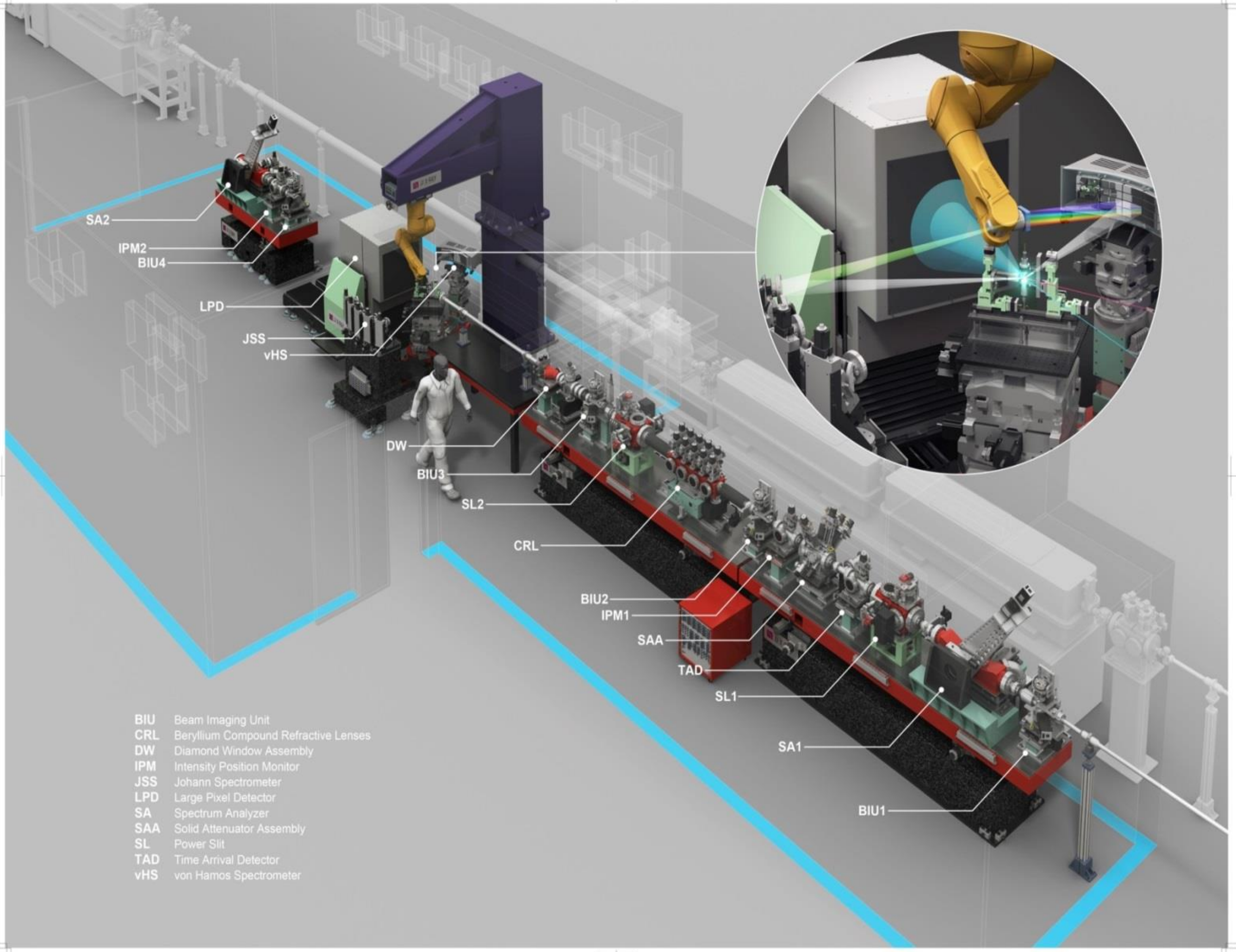


FXE instrument at European XFEL

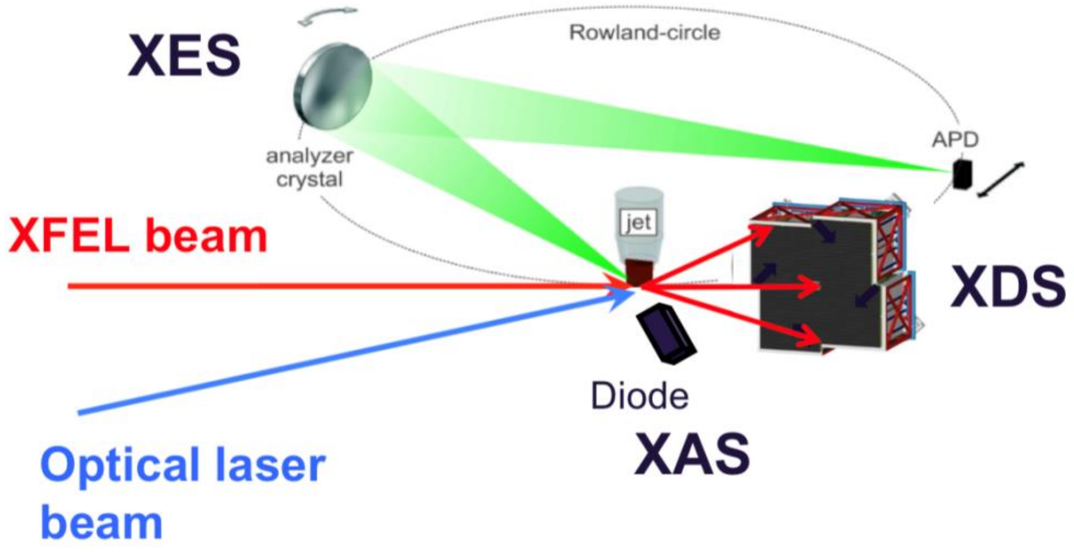
Ultrafast photo-induced processes in liquids and solids

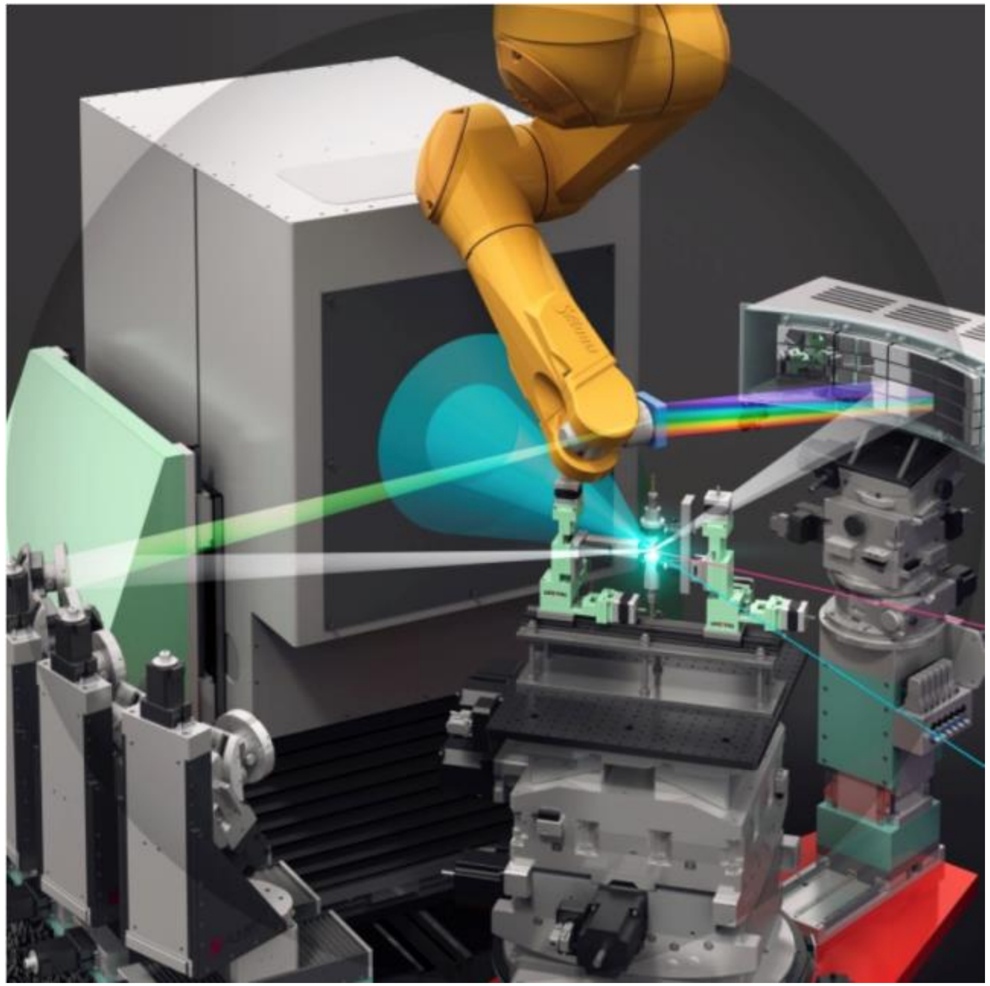
- Photo- & reaction chemistry
- Solid-state phase transitions





Combine X-ray Spectroscopy with X-ray Scattering tools in a single pump-probe experiment





- X-ray Absorption Spectroscopy (XAS)
- X-ray Emission Spectroscopy (XES)
- Resonant Inelastic X-ray Scattering (RIXS)
- X-ray Raman Scattering (XRS)
- Wide- Angle X-ray Scattering (WAXS)

FXE: versatile pump-probe instrument

Conclusions

- X-ray spectroscopic and scattering techniques have been successfully applied to study chemical reactions dynamics in solid and liquid environments
- The plethora of different observables can be connected in a single experiment deliver a more complete motion picture of the on-going chemical process
- Coherent wavepacket dynamics has been detected in XAS, XES and WAXS experiments revealing atomic movements during the ultrafast relaxation dynamics
- Combination of X-ray spectroscopy and X-ray scattering allows to track not only solute but also solvation cage and bulk solvent dynamics during the course of a chemical reaction.