In this work, we investigate the excited-state solute and solvation structure of [Ru(bpy)$_3$]$_2^{2+}$, [Fe(bpy)$_3$]$_2^{2+}$, [Fe(bmip)$_2$]$_2^{2+}$ and [Cu(phen)$_2$]$^+$ (bpy = 2,2'-bipyridine; bmip = 2,6-bis(3-methyl-imidazole-1-ylidine)-pyridine; phen = 1,10-phenanthroline) transition metal complexes (TMCs) in terms of solute-solvent radial distribution functions (RDFs) and evaluate the performance of some of the most popular partial atomic charge (PAC) methods for obtaining these RDFs by molecular dynamics (MD) simulations. To this end, we compare classical MD of a frozen solute in water and acetonitrile (ACN) with quantum mechanics/molecular mechanics Born-Oppenheimer molecular dynamics (QM/MM BOMD) simulations. The calculated RDFs show that the choice of a suitable PAC method is dependent on the coordination number of the metal, denticity of the ligands, and type of solvent. It is found that this selection is less sensitive for water than ACN. Furthermore, a careful choice of the PAC method should be considered for TMCs that exhibit a free direct coordination site, such as [Cu(phen)$_2$]$^+$. The results of this work show that fast classical MD simulations with ChelpG/RESP or CMS PACs can produce RDFs close to those obtained by QM/MM MD and thus, provide reliable solvation structures of TMCs to be used, e.g. in the analysis of scattering data.
Theoretical Evidence of Solvent-Mediated Excited-State Dynamics in a Functionalized Iron Sensitizer

The solvent-mediated excited-state dynamics of the COOH-functionalized Fe-carbene photosensitizer [Fe(bmicp)]$_2$$^{2+}$ (bmicp = 2,6-bis(3-methyl-imidazole-1-ylidine)-4-carboxy-pyridine) is studied by time-dependent density functional theory, as well as classical and quantum dynamics simulations. We demonstrate the crucial role of the polar acetonitrile solvent in stabilizing the metal-to-ligand charge transfer (MLCT) states of the investigated molecule using the conductor polarizable continuum model. This leads to dynamics that avoid sub-ps back electron transfer to the metal and an exceptionally long-lived 1MLCT state that does not undergo sub-ps $^1$MLCT $\rightarrow$ $^3$MLCT intersystem crossing as it is energetically isolated. We
identify two components of the excited-state solvent reorganization process: an initial rotation (∼300 fs) and diffusional
dynamics within the local cage surrounding the rotated solvent molecule (∼2 ps). Finally, it is found that the relaxation of
the solvent only slightly affects the excited-state population dynamics of [Fe(bmicp)₂]²⁺.

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Web of Science (2019): Indexed yes
BFI (2018): BFI-level 1
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Scopus rating (2017): CiteScore 4.58 SJR 2.135 SNIP 1.147
Web of Science (2017): Impact factor 4.484
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.48 SJR 1.964 SNIP 1.195
Web of Science (2016): Impact factor 4.536
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 4.68 SJR 1.886 SNIP 1.26
Web of Science (2015): Impact factor 4.509
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 5.08 SJR 2.032 SNIP 1.447
Web of Science (2014): Impact factor 4.772
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 5.14 SJR 2.143 SNIP 1.445
Web of Science (2013): Impact factor 4.835
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 4.98 SJR 2.529 SNIP 1.461
Web of Science (2012): Impact factor 4.814
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 4.92 SJR 2.339 SNIP 1.465
Web of Science (2011): Impact factor 4.805
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 2.462 SNIP 1.362
Web of Science (2010): Impact factor 4.524
How to Excite Nuclear Wavepackets into Electronically Degenerate States in Spin-Vibronic Quantum Dynamics Simulations

The excited-state dynamics of two functional Fe-carbene complexes, [Fe(bmip)₂]²⁺ (bmip = 2,6-bis(3-methyl-imidazole-1-ylidene)-pyridine) and [Fe(btibp)₂]²⁺ (btibp = 2,6-bis(3-tert-butyl-imidazole-1-ylidene)pyridine), are studied using the spin-vibronic model. In contrast to the usual projection of the ground state nuclear wavefunction onto an excited state surface, the dynamics are initiated by an explicit interaction term between the external time-dependent electric field (laser pulse) and the transition dipole moment of the molecule. The results show that the spin-vibronic model, as constructed directly from electronic structure calculations, exhibits erroneous, polarization-dependent relaxation dynamics stemming from artificial interference of coupled relaxation pathways. This is due to the lack of rotational invariance in the description of excitation into degenerate states. We introduce and discuss a correction using the spherical basis and complex transition dipole moments. This modification in the Hamiltonian leads to rotationally invariant excitation and produces polarization-independent population dynamics.

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Contributors: Pápai, M., Simmermacher, M., Penfold, T. J., Møller, K. B., Rozgonyi, T.
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BFI (2019): BFI-level 2
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 5.25 SJR 2.497 SNIP 1.476
Web of Science (2017): Impact factor 5.399
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Solution Structure and Ultrafast Vibrational Relaxation of the PtPOP Complex Revealed by ΔSCF-QM/MM Direct Dynamics Simulations

Recent ultrafast experiments have unveiled the time scales of vibrational cooling and decoherence upon photoexcitation of the diplatinum complex [Pt2(P2O5H2)4]4− in solvents. Here, we contribute to the understanding of the structure and dynamics of the lowest lying singlet excited state of the model photocatalyst by performing potential energy surface calculations and Born–Oppenheimer molecular dynamics simulations in the gas phase and in water. Solvent effects were treated using a multiscale quantum mechanics/molecular mechanics approach. Fast sampling was achieved with a modified version of delta self-consistent field implemented in the grid-based projector-augmented wave density functional theory code. The known structural parameters and the PESs of the first singlet and triplet excited states are correctly reproduced. Besides, the simulations deliver clear evidence that pseudorotation of the ligands in the excited state leads to symmetry lowering of the Pt2P8 core. Coherence decay of Pt–Pt stretching vibrations in solution was found to be governed by vibrational cooling, which is in agreement with previous ultrafast experiments. We also show that the flow of excess Pt–Pt vibrational energy is first directed toward vibrational modes involving the ligands, with the solvent favoring intramolecular vibrational energy redistribution. The results are supported by thorough vibrational analysis in terms of
generalized normal modes.

General information
State: Published
Organisations: Department of Chemistry, Technical University of Denmark
Contributors: Levi, G., Pápai, M. I., Henriksen, N. E., Dohn, A. O., Møller, K. B.
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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
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Scopus rating (2017): CiteScore 4.58 SJR 2.135 SNIP 1.147
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Scopus rating (2016): CiteScore 4.48 SJR 1.964 SNIP 1.195
Web of Science (2016): Impact factor 4.536
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 4.68 SJR 1.886 SNIP 1.26
Web of Science (2015): Impact factor 4.509
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 5.08 SJR 2.032 SNIP 1.447
Web of Science (2014): Impact factor 4.772
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 5.14 SJR 2.143 SNIP 1.445
Web of Science (2013): Impact factor 4.835
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 4.98 SJR 2.529 SNIP 1.461
Web of Science (2012): Impact factor 4.814
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 4.92 SJR 2.339 SNIP 1.465
Web of Science (2011): Impact factor 4.805
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 2.462 SNIP 1.362
Web of Science (2010): Impact factor 4.524
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Probing Transient Valence Orbital Changes with Picosecond Valence-to-Core X-ray Emission Spectroscopy
We probe the dynamics of valence electrons in photoexcited [Fe(terpy)2]2+ in solution to gain deeper insight into the Fe ligand bond changes. We use hard X-ray emission spectroscopy (XES), which combines element specificity and high penetration with sensitivity to orbital structure, making it a powerful technique for molecular studies in a wide variety of environments. A picosecond-time-resolved measurement of the complete Ls X-ray emission spectrum captures the transient photoinduced changes and includes the weak valence-to-core (vtc) emission lines that correspond to transitions from occupied valence orbitals to the nascent core-hole. Vtc-XES offers particular insight into the molecular orbitals directly involved in the light-driven dynamics; a change in the metal ligand overlap results in an intensity reduction and a blue energy shift in agreement with our theoretical calculations and more subtle features at the highest energies reflect changes in the frontier orbital populations.

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BFI (2019): BFI-level 1
Web of Science (2019): Indexed yes
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 4.58 SJR 2.135 SNIP 1.147
Web of Science (2017): Impact factor 4.484
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.48 SJR 1.964 SNIP 1.195
Web of Science (2016): Impact factor 4.536
Web of Science (2016): Indexed yes
Characterizing the Solvated Structure of Photoexcited \([\text{Os(terpy)}_2]^{2+}\) with X-ray Transient Absorption Spectroscopy and DFT Calculations

Characterizing the geometric and electronic structures of individual photoexcited dye molecules in solution is an important step towards understanding the interfacial properties of photo-active electrodes. The broad family of "red sensitizers" based on osmium(II) polypyridyl compounds often undergoes small photo-induced structural changes which are challenging to characterize. In this work, X-ray transient absorption spectroscopy with picosecond temporal resolution is
employed to determine the geometric and electronic structures of the photoexcited triplet state of [Os(terpy)$_2$]$^{2+}$ (terpy: 2,2':6',2''-terpyridine) solvated in methanol. From the EXAFS analysis, the structural changes can be characterized by a slight overall expansion of the first coordination shell [OsN$_6$]. DFT calculations supports the XTA results. They also provide additional information about the nature of the molecular orbitals that contribute to the optical spectrum (with TD-DFT) and the near-edge region of the X-ray spectra.

**General information**

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Organisations: Department of Chemistry, Tianjin Polytechnic University, Deutsches Elektronen-Synchrotron, Argonne National Laboratory
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BFI (2019): BFI-level 1
Web of Science (2019): Indexed yes
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
Scopus rating (2017): CiteScore 3.27 SJR 0.855 SNIP 1.146
Web of Science (2017): Impact factor 3.098
Web of Science (2016): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.09 SJR 0.825 SNIP 1.257
Web of Science (2016): Impact factor 2.861
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 2.65 SJR 0.57 SNIP 1.164
Web of Science (2015): Impact factor 2.465
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.62 SJR 0.738 SNIP 1.3
Web of Science (2014): Impact factor 2.416
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 2.61 SJR 0.719 SNIP 1.268
Web of Science (2013): Impact factor 2.095
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 2.87 SJR 0.792 SNIP 1.363
Web of Science (2012): Impact factor 2.428
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 2.54 SJR 0.72 SNIP 1.119
Web of Science (2011): Impact factor 2.386
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Effect of tert-Butyl Functionalization on the Photoexcited Decay of a Fe(II)-N-Heterocyclic Carbene Complex

Understanding and subsequently being able to manipulate the excited-state decay pathways of functional transition-metal complexes is of utmost importance in order to solve grand challenges in solar energy conversion and data storage. Herein, we perform quantum chemical calculations and spin-vibronic quantum dynamics simulations on the Fe-N-heterocyclic carbene complex, [Fe(btbip)2]2+ (btbip = 2,6-bis(3-tert-butyl-imidazole-1-ylidene)pyridine). The results demonstrate that a relatively minor structural change compared to its parent complex, [Fe(bmip)2]2+ (bmip = 2,6-bis(3-methyl-imidazole-1-ylidene)pyridine), completely alters the excited-state relaxation. Ultrafast deactivation of the initially excited metal-to-ligand charge transfer (1,3MLCT) states occurs within 350 fs. In contrast to the widely adopted mechanism of Fe(II) photophysics, these states decay into close-lying singlet metal-centered (1MC) states. This occurs because the tert-butyl functionalization stabilizes the 1MC states, enabling the 1,3MLCT → 1MC population transfer to occur close to the Franck-Condon geometry, making the conversion very efficient. Subsequently, a spin cascade occurs within the MC manifold, leading to the population of triplet and quintet MC states. These results will inspire highly involved ultrafast experiments performed at X-ray free electron lasers and shall pave the way for the design of novel high-efficiency transition-metal-based functional molecules.

Bibliographical note
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BFI (2019): BFI-level 1
Elucidating the Ultrafast Dynamics of Photoinduced Charge Separation in Metalloporphyrin-Fullerene Dyads Across the Electromagnetic Spectrum

Metalloporphyrins are prominent building blocks in the synthetic toolbox of advanced photodriven molecular devices. When the central ion is paramagnetic, the relaxation pathways within the manifold of excited states are highly intricate so that unravelling the intramolecular energy and electron transfer processes is usually a very complex task. This fact is critically hampering the development of applications based on the enhanced coupling offered by the electronic exchange interaction. In this work, the dynamics of charge separation in a copper porphyrin-fullerene are studied with several complementary spectroscopic tools across the electromagnetic spectrum (from near-infrared to X-ray wavelengths), each of them providing specific diagnostics. Correlating the various rates clearly demonstrates that the lifetime of the photoinduced charge-separated state exceeds by about 10-fold that of the isolated photoexcited CuII porphyrin. As revealed by the spectral modifications in the XANES region, this stabilization is accompanied by a transient change in covalency around the CuII center, which is induced by an enhanced interaction with the C60 moiety. This experimental finding is further confirmed by state-of-the-art calculations using DFT and TD-DFT including dispersion effects that explain the electrostatic and structural origins of this interaction, as the CuII porphyrin becomes ruffled and approaches closer to the fullerene in the charge-separated state. From a methodological point of view, these results exemplify the potential of multielectron excitation features in transient X-ray spectra as future diagnostics of subfemtosecond electronic dynamics. From a practical point of view, this work is paving the way for elucidating out-of-equilibrium electron transfer events coupled to magnetic interaction processes on their intrinsic time-scales.

General information

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BFI (2019): BFI-level 1
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 4.58 SJR 2.135 SNIP 1.147
Web of Science (2017): Impact factor 4.484
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.48 SJR 1.964 SNIP 1.195
Web of Science (2016): Impact factor 4.536
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 4.68 SJR 1.886 SNIP 1.26
Web of Science (2015): Impact factor 4.509
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
We study the structural dynamics of photoexcited \([\text{Co(terpy)}_2]^2+\) in an aqueous solution with ultrafast x-ray diffuse scattering experiments conducted at the Linac Coherent Light Source. Through direct comparisons with density functional theory calculations, our analysis shows that the photoexcitation event leads to elongation of the Co-N bonds, followed by coherent Co-N bond length oscillations arising from the impulsive excitation of a vibrational mode dominated by the symmetrical stretch of all six Co-N bonds. This mode has a period of 0.33 ps and decays on a subpicosecond time scale. We find that the equilibrium bond-elongated structure of the high spin state is established on a single-picosecond time scale and that this state has a lifetime of ~7 ps.
High-Efficiency Iron Photosensitizer Explained with Quantum Wavepacket Dynamics

Fe(II) complexes have long been assumed unsuitable as photosensitizers because of their low-lying nonemissive metal centered (MC) states, which inhibit electron transfer. Herein, we describe the excited-state relaxation of a novel Fe(II) complex that incorporates N-heterocyclic carbene ligands designed to destabilize the MC states. Using first-principles quantum nuclear wavepacket simulations we achieve a detailed understanding of the photoexcited decay mechanism, demonstrating that it is dominated by an ultrafast intersystem crossing from \(^1\)MLCT–\(^3\)MLCT proceeded by slower kinetics associated with the conversion into the \(^3\)MC states. The slowest component of the \(^3\)MLCT decay, important in the context of photosensitizers, is much longer than related Fe(II) complexes because the population transfer to the \(^3\)MC states occurs in a region of the potential where the energy gap between the \(^3\)MLCT and \(^3\)MC states is large, making the population transfer inefficient.

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Organisations: Department of Chemistry, Newcastle University, Hungarian Academy of Sciences
Contributors: Pápai, M. I., Vankó, G., Rozgonyi, T., Penfold, T. J.
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BFI (2019): BFI-level 2
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 8.37 SJR 4.667 SNIP 1.595
Web of Science (2017): Impact factor 8.709
Observing Solvation Dynamics with Simultaneous Femtosecond X-ray Emission Spectroscopy and X-ray Scattering

In liquid phase chemistry dynamic solute solvent interactions often govern the path, ultimate outcome, and efficiency of chemical reactions. These steps involve many-body movements on subpicosecond time scales and thus ultrafast structural tools capable of capturing both intramolecular electronic and structural changes, and local solvent structural changes are desired. We have studied the intra- and intermolecular dynamics of a model chromophore, aqueous $[\text{Fe(bpy)}_2]^2+$, with complementary X-ray tools in a single experiment exploiting intense XFEL radiation as a probe. We monitored the ultrafast structural rearrangement of the solute with X-ray emission spectroscopy, thus establishing time zero for the ensuing X-ray diffuse scattering analysis. The simultaneously recorded X-ray diffuse scattering attens reveal slower subpicosecond dynamics triggered by the intramolecular structural dynamics of the photoexcited solute. By simultaneous combination of both methods only, we can extract new information about the solvation dynamic processes unfolding...
during the first picosecond (ps). The measured bulk solvent density increase of 0.2% indicates a dramatic change of the solvation shell around each photoexcited solute, confirming previous ab initio molecular dynamics simulations. Structural changes in the aqueous solvent associated with density and temperature changes occur with similar to 1 ps time constants, characteristic for structural dynamics in water. This slower time scale of the solvent response allows us to directly observe the structure of the excited solute molecules well before the solvent contributions become dominant.

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Web of Science (2019): Indexed yes
BFI (2018): BFI-level 1
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BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 3.13 SJR 1.331 SNIP 1.015
Web of Science (2017): Impact factor 3.146
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.03 SJR 1.345 SNIP 1.012
Web of Science (2016): Impact factor 3.177
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 3.25 SJR 1.335 SNIP 1.076
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 3.28 SJR 1.449 SNIP 1.138
Web of Science (2014): Impact factor 3.302
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 3.53 SJR 1.504 SNIP 1.202
Web of Science (2013): Impact factor 3.377
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 3.66 SJR 1.943 SNIP 1.256
Web of Science (2012): Impact factor 3.607
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 3.62 SJR 1.801 SNIP 1.223
Web of Science (2011): Impact factor 3.696
Probing spin-vibronic dynamics using femtosecond X-ray spectroscopy

Ultrafast pump-probe spectroscopy within the X-ray regime is now possible owing to the development of X-ray Free Electrons Lasers (X-FELs) and is opening new opportunities for the direct probing of femtosecond evolution of the nuclei, the electronic and spin degrees of freedom. In this contribution we use wavepacket dynamics of the photoexcited decay of a new Fe(II) complex, [Fe(bmip)]^{2+} (bmip = 2,6-bis(3-methyl-imidazole-1-ylidine)pyridine), to simulate the experimental observables associated with femtosecond Fe K-edge X-ray Absorption Near-Edge Structure (XANES) and X-ray emission (XES) spectroscopy. We show how the evolution of the nuclear wavepacket is translated into the spectroscopic signal and the sensitivity of these approaches for following excited state dynamics.
Ratings:
BFI (2019): BFI-level 1
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 3.03 SJR 1.458 SNIP 0.868
Web of Science (2017): Impact factor 3.427
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.07 SJR 1.524 SNIP 0.903
Web of Science (2016): Impact factor 3.588
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 3.54 SJR 1.489 SNIP 1.042
Web of Science (2015): Impact factor 3.544
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 3.79 SJR 1.732 SNIP 1.274
Web of Science (2014): Impact factor 4.606
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 3.65 SJR 1.645 SNIP 1.149
Web of Science (2013): Impact factor 4.194
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 3.24 SJR 1.751 SNIP 0.938
Web of Science (2012): Impact factor 3.821
ISI indexed (2012): ISI indexed no
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 3.92 SJR 1.93 SNIP 1.232
Web of Science (2011): Impact factor 5
ISI indexed (2011): ISI indexed no
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.755 SNIP 1.231
Web of Science (2010): Impact factor 4.538
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.85 SNIP 1.168
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.819 SNIP 1.299
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.914 SNIP 1.315
Scopus rating (2006): SJR 1.548 SNIP 1.268
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.655 SNIP 1.167
Scopus rating (2004): SJR 1.251 SNIP 1.093
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.231 SNIP 1.013
Scopus rating (2002): SJR 1.508 SNIP 1.033
Scopus rating (2001): SJR 1.783 SNIP 0.967
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 1.153 SNIP 1.199
Web of Science (2000): Indexed yes
Detailed Characterization of a Nanosecond-Lived Excited State: X-ray and Theoretical Investigation of the Quintet State in Photoexcited [Fe(terpy)(2)](2+)

Theoretical predictions show that depending on the populations of the Fe 3d(xy), 3d(xz), and 3d(yz) orbitals two possible quintet states can exist for the high-spin state of the photoswitchable model system [Fe(terpy)(2)](2+). The differences in the structure and molecular properties of these B-5(2) and E-5 quintets are very small and pose a substantial challenge for experiments to resolve them. Yet for a better understanding of the physics of this system, which can lead to the design of novel molecules with enhanced photoswitching performance, it is vital to determine which high-spin state is reached in the transitions that follow the light excitation. The quintet state can be prepared with a short laser pulse and can be studied with cutting-edge time-resolved X-ray techniques. Here we report on the application of an extended set of X-ray spectroscopy and scattering techniques applied to investigate the quintet state of [Fe(terpy)(2)](2+) 80 ps after light excitation. High-quality X-ray absorption, nonresonant emission, and resonant emission spectra as well as X-ray diffuse scattering data clearly reflect the formation of the high-spin state of the [Fe(terpy)(2)](2+) molecule; moreover, extended X-ray absorption fine structure spectroscopy resolves the Fe-ligand bond-length variations with unprecedented bond-length accuracy in time-resolved experiments. With ab initio calculations we determine why, in contrast to most related systems, one configurational mode is insufficient for the description of the low-spin (LS)-high-spin (HS) transition. We identify the electronic structure origin of the differences between the two possible quintet modes, and finally, we unambiguously identify the formed quintet state as 5E, in agreement with our theoretical expectations.
X-ray spectroscopies, when combined in laser-pump, X-ray-probe measurement schemes, can be powerful tools for tracking the electronic and geometric structural changes that occur during the course of a photoinitiated chemical reaction. X-ray absorption spectroscopy (XAS) is considered an established technique for such measurements, and X-ray emission spectroscopy (XES) of the strongest core-to-core emission lines (K alpha and K beta) is now being utilized. Flux demanding valence-to-core XES promises to be an important addition to the time-resolved spectroscopic toolkit. In this paper we present measurements and density functional theory calculations on laser-excited, solution-phase ferrocyanide
that demonstrate the feasibility of valence-to-core XES for time-resolved experiments. We discuss technical improvements that will make valence-to-core XES a practical pump-probe technique.

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BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 4.92 SJR 2.339 SNIP 1.465
Web of Science (2011): Impact factor 4.805
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 2.462 SNIP 1.362
Web of Science (2010): Impact factor 4.524
Visualizing the non-equilibrium dynamics of photoinduced intramolecular electron transfer with femtosecond X-ray pulses

Ultrafast photoinduced electron transfer preceding energy equilibration still poses many experimental and conceptual challenges to the optimization of photoconversion since an atomic-scale description has so far been beyond reach. Here we combine femtosecond transient optical absorption spectroscopy with ultrafast X-ray emission spectroscopy and diffuse X-ray scattering at the SACLA facility to track the non-equilibrated electronic and structural dynamics within a bimetallic donor–acceptor complex that contains an optically dark centre. Exploiting the 100-fold increase in temporal resolution as compared with storage ring facilities, these measurements constitute the first X-ray-based visualization of a non-equilibrated intramolecular electron transfer process over large interatomic distances. Experimental and theoretical results establish that mediation through electronically excited molecular states is a key mechanistic feature. The present study demonstrates the extensive potential of femtosecond X-ray techniques as diagnostics of non-adiabatic electron transfer processes in synthetic and biological systems, and some directions for future studies, are outlined.

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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Center for Atomic-scale Materials Design, Department of Chemistry, Physical and Biophysical Chemistry, Lund University, University of Copenhagen, Hungarian Academy of Sciences, High Energy Accelerator Research Organization, The Hamburg Centre for Ultrafast Imaging, European XFEL, Argonne National Laboratory, RIKEN, Japan Synchrotron Radiation Research Institute
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Watching the dynamics of electrons and atoms at work in solar energy conversion

The photochemical reactions performed by transition metal complexes have been proposed as viable routes towards solar energy conversion and storage into other forms that can be conveniently used in our everyday applications. In order to develop efficient materials, it is necessary to identify, characterize and optimize the elementary steps of the entire process on the atomic scale. To this end, we have studied the photoinduced electronic and structural dynamics in two heterobimetallic ruthenium–cobalt dyads, which belong to the large family of donor–bridge–acceptor systems. Using a combination of ultrafast optical and X-ray absorption spectroscopies, we can clock the light-driven electron transfer processes with element and spin sensitivity. In addition, the changes in local structure around the two metal centers are monitored. These experiments show that the nature of the connecting bridge is decisive for controlling the forward and the backward electron transfer rates, a result supported by quantum chemistry calculations. More generally, this work illustrates how ultrafast optical and X-ray techniques can disentangle the influence of spin, electronic and nuclear factors on the intramolecular electron transfer process. Finally, some implications for further improving the design of bridged sensitizer-catalysts utilizing the presented methodology are outlined.
Exceptional Excited-State Lifetime of an Iron(II)-N-Heterocyclic Carbene Complex Explained

Earth-abundant transition-metal complexes are desirable for sensitizers in dye-sensitized solar cells or photocatalysts. Iron is an obvious choice, but the energy level structure of its typical polypyridyl complexes, featuring low-lying metal-centered states, has made such complexes useless as energy converters. Recently, we synthesized a novel iron-N-heterocyclic carbene complex exhibiting a remarkable 100-fold increase of the lifetime compared to previously known iron(II) complexes. Here, we rationalize the measured excited-state dynamics with DFT and TD-DFT calculations. The calculations show that the exceptionally long excited-state lifetime (similar to 9 ps) is achieved for this Fe complex through a significant destabilization of both triplet and quintet metal-centered scavenger states compared to other Fe complexes. In addition, a shallow (MLCT)-M-3 potential energy surface with a low-energy transition path from the (MLCT)-M-3 to (MC)-M-3 and facile crossing from the (MC)-M-3 state to the ground state are identified as key features for the excited-state deactivation.

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BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 8.37 SJR 4.667 SNIP 1.595
Web of Science (2017): Impact factor 8.709
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 8.18 SJR 4.602 SNIP 1.651
Ferromagnetic Coupling in an Fe[C(SiMe3)(3)](2)/Ferrihydrite Hetero-Mixture Molecular Magnet: Ferromagnetic Coupling in Fe[C(SiMe3)(3)](2)/Ferrihydrite

Magnetization and low temperature in-field Fe-57 Mossbauer spectroscopy measurements have been performed on a Fe[C(SiMe3)(3)](2)/ferrihydrite hetero-mixture. The results indicate the presence of ferromagnetic coupling of magnetic moments involving Fe[C(SiMe3)(3)](2) with a hyperfine magnetic field of about 151 T, attributable mainly to the non-frozen atomic orbital contribution. The present findings show the sensitivity of single-ion molecular magnets to local alterations of their lattice-environment and might explain and reconcile some of the differences found in the literature for the observed bulk magnetic properties of the title Fe[C(SiMe3)(3)](2) compound.
On Predicting Mössbauer Parameters of Iron-Containing Molecules with Density-Functional Theory

The performance of six frequently used density functional theory (DFT) methods (RPBE, OLYP, TPSS, B3LYP, B3LYP*, and TPSSh) in the prediction of Mössbauer isomer shifts(δ) and quadrupole splittings (ΔEQ) is studied for an extended and diverse set of Fe complexes. In addition to the influence of the applied density functional and the type of the basis set, the effect of the environment of the molecule, approximated with the conducting-like screening solvation model (COSMO) on the computed Mössbauer parameters, is also investigated. For the isomer shifts the COSMO-B3LYP method is found to provide accurate δ values for all 66 investigated complexes, with a mean absolute error (MAE) of 0.05 mm s(-1) and a maximum deviation of 0.12 mm s(-1). Obtaining accurate ΔEQ values presents a bigger challenge; however, with the selection of an appropriate DFT method, a reasonable agreement can be achieved between experiment and theory. Identifying the various chemical classes of compounds that need different treatment allowed us to construct a recipe for ΔEQ calculations; the application of this approach yields a MAE of 0.12 mm s(-1) (7% error) and a maximum deviation of 0.55 mm s(-1) (17% error). This accuracy should be sufficient for most chemical problems that concern Fe complexes. Furthermore, the reliability of the DFT approach is verified by extending the investigation to chemically relevant case studies which include geometric isomerism, phase transitions induced by variations of the electronic structure (e.g., spin crossover and inversion of the orbital ground state), and the description of electronically degenerate triplet and quintet states. Finally, the immense and often unexploited potential of utilizing the sign of the ΔEQ in characterizing distortions or in identifying the appropriate electronic state at the assignment of the spectral lines is also shown.

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BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 5.25 SJR 2.497 SNIP 1.476
On the sensitivity of hard X-ray spectroscopies to the chemical state of Br

The sensitivity of the 1s X-ray emission and high-energy-resolution fluorescence-detected X-ray absorption spectroscopies (XES and HERFD-XAS) to resolve the variations in the chemical state (electronic structure and local coordination) of Br has been investigated for a selected set of compounds including NaBrO$_3$, NH$_4$Br and C$_2$H$_4$Br$_2$ (1,2-
dibromoethane). For the Br K-edge XAS, employing the HERFD mode significantly increases the energy resolution, which demonstrates that with a crystal spectrometer used as a detector the absorption technique becomes a more powerful analytical tool. In the case of XES, the experimental results as well as the density functional theory (DFT) modeling both show that the chemical sensitivity of the main 1s diagram emission lines (Kα_{1,2} and Kβ_{1,3}) is rather limited. However, the valence-to-core (Kβ_2) region of XES displays significant shape and intensity variations, as expected for transitions having the same final states as those of photoemission spectroscopy. The spectra are in good agreement with the molecular orbital description delivered by DFT calculations. Calculations for an extended series of Br compounds confirm that valence-to-core XES can serve as a probe for chemical analysis, and, being a hard X-ray photon-in/photon-out technique, it is particularly well-suited for in situ investigations of molecular transformations, even on the ultrafast time scales down to femtosecond time resolution.

**General information**

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Organisations: Hungarian Academy of Sciences, Paul Scherrer Institute
Contributors: Bordage, A., Pápai, M. I., Sas, N. S., Szlachetko, J., Nachtegaal, M., Vanko, G.
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- Scopus rating (2017): CiteScore 4.04 SJR 1.686 SNIP 1.089
- Web of Science (2017): Impact factor 3.906
- Web of Science (2017): Indexed yes
- BFI (2016): BFI-level 2
- Scopus rating (2016): CiteScore 4.06 SJR 1.685 SNIP 1.113
- Web of Science (2016): Impact factor 4.123
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 2
- Scopus rating (2015): CiteScore 4.45 SJR 1.725 SNIP 1.205
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 2
- Scopus rating (2014): CiteScore 4.29 SJR 1.771 SNIP 1.239
- Web of Science (2014): Impact factor 4.493
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 2
- Scopus rating (2013): CiteScore 4.05 SJR 1.72 SNIP 1.207
- Web of Science (2013): Impact factor 4.198
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- BFI (2012): BFI-level 2
- Scopus rating (2012): CiteScore 3.67 SJR 1.921 SNIP 1.177
- Web of Science (2012): Impact factor 3.829
- ISI indexed (2012): ISI indexed yes
- Web of Science (2012): Indexed yes
- BFI (2011): BFI-level 2
- Scopus rating (2011): CiteScore 3.6 SJR 1.707 SNIP 1.19
Toward Highlighting the Ultrafast Electron Transfer Dynamics at the Optically Dark Sites of Photocatalysts

Building a detailed understanding of the structure–function relationship is a crucial step in the optimization of molecular photocatalysts employed in water splitting schemes. The optically dark nature of their active sites usually prevents a complete mapping of the photoinduced dynamics. In this work, transient X-ray absorption spectroscopy highlights the electronic and geometric changes that affect such a center in a bimetallic model complex. Upon selective excitation of the ruthenium chromophore, the cobalt moiety is reduced through intramolecular electron transfer and undergoes a spin flip accompanied by an average bond elongation of 0.20 ± 0.03 Å. The analysis is supported by simulations based on density functional theory structures (B3LYP*/TZVP) and FEFF 9.0 multiple scattering calculations. More generally, these results exemplify the large potential of the technique for tracking elusive intermediates that impart unique functionalities in photochemical devices.

General information
State: Published
Organisations: Department of Physics, Department of Chemistry, Physical and Biophysical Chemistry, Lund University, Argonne National Laboratory, Hungarian Academy of Sciences, European XFEL, SLAC National Accelerator Laboratory, Uppsala University, University of Copenhagen, European Synchrotron Radiation Facility
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Theoretical Investigation of the Electronic Structure of Fe(II) Complexes at Spin-State Transitions

The electronic structure relevant to low spin (LS) ↔ high spin (HS) transitions in Fe(II) coordination compounds with a FeN_6 core are studied. The selected [Fe(tz)_6]^{2+} (1) (tz = 1H-tetrazole), [Fe(bipy)_3]^{2+} (2) (bipy = 2,2'-bipyridine), and [Fe(terpy)_2]^{3+} (3) (terpy = 2,2':6',2''-terpyridine) complexes have been actively studied experimentally, and with their respective mono-, bi-, and tridentate ligands, they constitute a comprehensive set for theoretical case studies. The methods in this work include density functional theory (DFT), time-dependent DFT (TD-DFT), and multiconfigurational second order perturbation theory (CASPT2). We determine the structural parameters as well as the energy splitting of the LS-HS states (ΔE_{LS-HS}) applying the above methods and comparing their performance. We also determine the potential energy curves representing the ground and low energy excited singlet, triplet, and quintet d(6) states along the mode(s) that connect the LS and HS states. The results indicate that while DFT is well suited for the prediction of structural parameters, an accurate multiconfigurational approach is essential for the quantitative determination of ΔE_{LS-HS}. In addition, a good qualitative agreement is found between the TD-DFT and CASPT2 potential energy curves. Although the TD-DFT results might differ in some respect (in our case, we found a discrepancy at the triplet states), our results suggest that this approach, with due care, is very promising as an alternative for the very expensive CASPT2 method. Finally, the two-dimensional (2D) potential energy surfaces above the plane spanned by the two relevant configuration coordinates in [Fe(terpy)_2]^{3+} were computed at both the DFT and CASPT2 levels. These 2D surfaces indicate that the singlet-triplet and triplet-quintet states are separated along different coordinates, i.e., different vibration modes. Our results confirm that in contrast to the case of complexes with mono- and bidentate ligands, the singlet-quintet transitions in [Fe(terpy)_2]^{3+} cannot be described using a single configuration coordinate.

General information

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Scopus rating (2017): CiteScore 5.25 SJR 2.497 SNIP 1.476
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BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 5.65 SJR 2.702 SNIP 1.643
Web of Science (2015): Impact factor 5.301
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
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Web of Science (2014): Impact factor 5.498
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ISI indexed (2013): ISI indexed yes
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BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 5.34 SJR 2.784 SNIP 1.614
Web of Science (2012): Impact factor 5.389
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
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Web of Science (2011): Impact factor 5.215
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.431 SNIP 1.457
Web of Science (2010): Impact factor 5.138
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.685 SNIP 1.297
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 2.486 SNIP 1.222
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Web of Science (2007): Indexed yes
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**Projects:**

**Atomistic Mechanisms of Functional Molecules**
Abedi, M., PhD Student, Department of Chemistry
Møller, K. B., Main Supervisor, Department of Chemistry
Henriksen, N. E., Supervisor, Department of Chemistry
Pápai, M. I., Supervisor, Department of Chemistry
Samfinansieret - Andet
01/02/2016 → 16/05/2019
Award relations: Atomistic Mechanisms of Functional Molecules
Project: PhD