Max-Planck-Institut für
Struktur und Dynamik der Materie
Max Planck Institute for the Structure and Dynamics of Matter

## IMPRS UFAST Call for PhD applications 2020/2021

# Ultrafast X-ray tracking of solvent-mediated charge transfer and metallophilicity in polynuclear transition metal complexes

**D. Khakhulin**

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| **Title of PhD Project** | **Ultrafast X-ray tracking of solvent-mediated charge transfer and metallophilicity in polynuclear transition metal complexes** |
| **Type** | Experimental |
| **Supervisor(s)** | Dr. Dmitry Khakhulin, Dr. Christopher Milne |
| **Affiliation(s):** | European XFEL |
| **Number of positions:** | 1 |
| **Abstract:** | In this project, we proposed to employ ultrafast X-ray scattering as well as optical and X-ray spectroscopies to investigate fundamental light-driven phenomena in polynuclear transition metal complexes relevant for energy conversion, photocatalysis, chemical sensing and bio-imaging. This experimental project will focus on detailed understanding of the global structural and electronic origins of enhances efficiency of charge transfer, metallophilic interactions and their cooperativity in transient electronically excited states. In particular, the influence of the surrounding environment, i.e. the solvation shell in solution systems, has been shown to greatly influence the metallophilicity in gold dimer complexes as it substantially modifies the potential energy landscape of the solute facilitating charge transfer processes.<br>The main goal of the project is to be able to independently track with femtosecond temporal resolution the most relevant dynamic degrees of freedom throughout the formation and relaxation of the excited stated governing the photo-reactivity under investigation. These transient degrees of freedom mainly include the high resolution structure of the solute and the solvation shell as well as the electronic configuration. We propose taking full advantage of the high energy X-ray photons available at the European XFEL and in particular the X-ray scattering and spectroscopic capabilities of the FXE instrument to perform these studies.<br>The project will commence with studying metallophilicity in solvated dimers of gold, silver and platinum towards optimizing this type of interaction. We will then continue extending the study to more earth abundant 3d metal (Cu, Ni, Co, Fe) compounds exhibiting electron transfer, also increasing their nuclearity to e.g. squares and other grid-like geometries. |
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