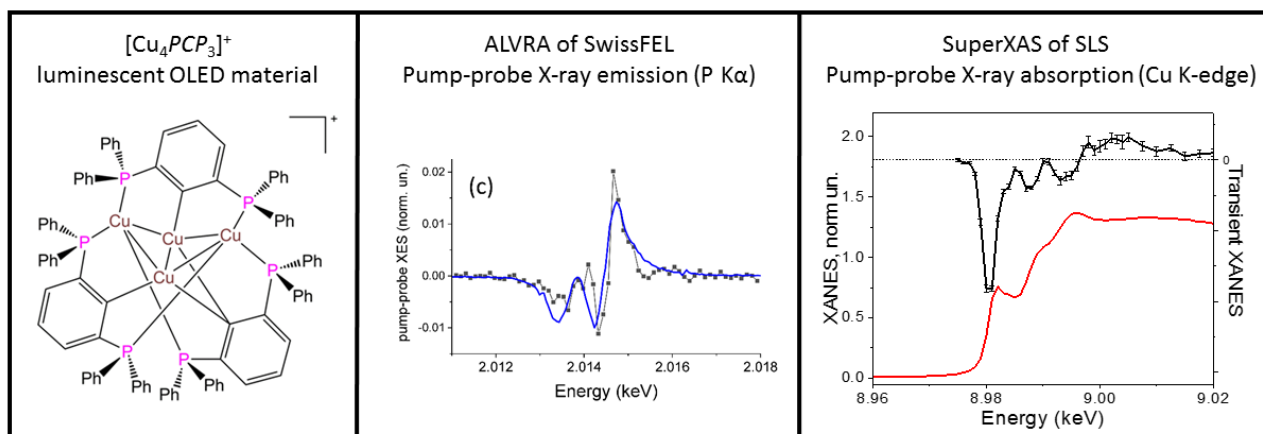


Pump-probe X-ray Experiments to Probe Excited State of Cu-based Complex for Organic Light-emitting Diodes

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The results of pilot pump-probe X-ray emission experiment at ALVRA endstation of SwissFEL, combined with pump-probe measurements in the microsecond time range at SuperXAS beamline of SLS and wide-angle X-ray scattering data acquired at ID09 of ESRF will be presented [1]. We have investigated the charge transfer and structural rearrangements in an organometallic multicore Cu complex, which is promising material for organic light-emitting diodes. We found that excitation leads to delocalized charge movement from C- and P- coordinated Cu sites and from phosphorus to phenyl rings. This is accompanied by the small rearrangement of the Cu core with 0.05 Å increase of the shortest Cu-Cu distance. The organometallic small-cluster strategy with robust Cu-C bonds and metallophilic Cu-Cu interactions is efficient to provide structural rigidity of luminophores. Obtained experimental data can be used to verify computational methods for the rational development of new luminescent materials for OLEDs.



- [1] G. Smolentsev, C. J. Milne, A. Guda, K. Haldrup, J. Szlachetko, N. Azzaroli, C. Cirelli, G. Knopp, R. Bohinc, S. Menzi, G. Pamfilidis, D. Gashi, M. Beck, A. Mozzanica, D. James, C. Bacellar, G. F. Mancini, A. Tereshchenko, V. Shapovalov, W. M. Kwiatak, J. Czapla-Masztafiak, A. Cannizzo, M. Gazzetto, M. Sander, M. Levantino, V. Kabanova, E. Rychagova, S. Ketkov, M. Olaru, J. Beckmann, M. Vogt *Nature Communications* (2020) 11, 2131.