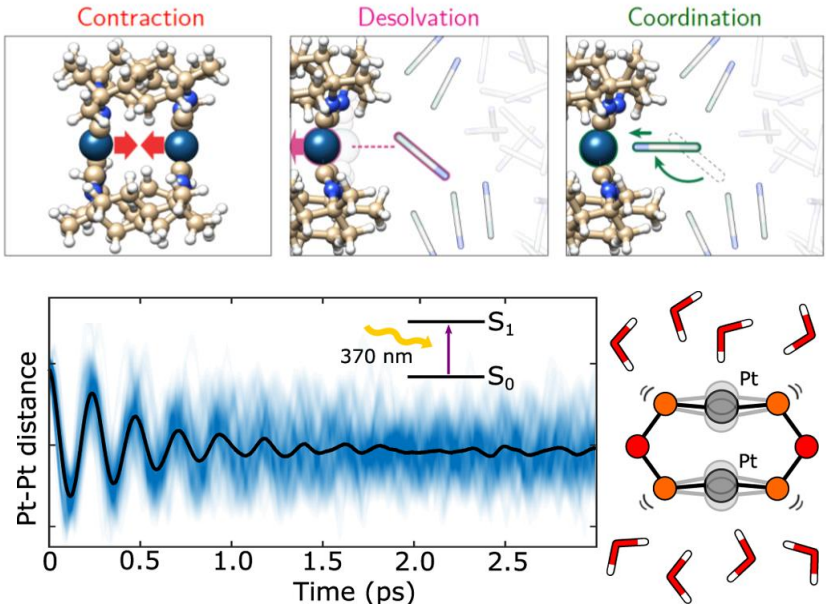
Real-time mapping of photo-induced bond formation and accompanying relaxation dynamics

Klaus Braagaard Møller

Department of Chemistry, Technical University of Denmark, 2800 Kgs. Lyngby, Denmark
kbmo@kemi.dtu.dk

Time-resolved X-ray scattering is used for investigations of structural dynamics in real time. However, analysis and interpretation of the experimental outcomes require support from theory and detailed atomistic simulations. In this contribution, we build on our developments of the theory behind time-resolved x-ray scattering [1,2] and illustrate how we have used computer simulations to assist pico- and femtosecond scattering experiments for mapping of ground- and excited-state bond formation and accompanying solute and solvent relaxations in solvated I_2 [3], $[Ir_2(Dimen)_4]^{2+}$ [4,5], and $[Pt_2(P_2O_5H_2)_4]^{4-}$ [6,7].



Our QM/MM BOMD code was used to model ground-state properties as well as the ultrafast photo-induced bond formation between the metals and the subsequent intra- and inter-molecular relaxation dynamics in solvated $[Ir_2(Dimen)_4]^{2+}$ (top) and $[Pt_2(P_2O_5H_2)_4]^{4-}$ (bottom).

References

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