Structural Dynamics

Preface to the special issue: Selected papers from the 5th International Conference on Ultrafast Structural Dynamics

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This special issue collects selected papers from participants of the 5th International Conference on Ultrafast Structural Dynamics (ICUSD 2019), which was held at KAIST, Daejeon, South Korea, on June 25–28, 2019. ICUSD 2019 succeeded previous ICUSD conferences held at Trieste, Italy in 2017, at Zurich, Switzerland in 2015, at Berlin, Germany in 2012, and at Lausanne, Switzerland in 2010, and it is the first one held outside Europe.

ICUSD 2019 brought together researchers in the fields of molecular structural dynamics, femtoscience, and ultrafast phenomena and provided opportunities to share ideas and discuss the latest developments of theory and experiment aimed at understanding and probing of structural dynamics in physics, chemistry, biology, and materials science. Researchers in related fields were also invited. Ultrafast structural dynamics span a variety of research communities, who have interest in visualizing the dynamics of atomic/molecular assemblies in space (sub-Å) and time (femtosecond) at the atomic scale using a variety of experimental techniques such as ultrafast electron/x-ray diffraction, scattering, spectroscopy, time-resolved x-ray/electron microscopy for dynamic imaging of matter, ultrafast multidimensional vibrational/electronic spectroscopies, x-ray/electron serial crystallography, and ultrafast Raman/IR/optical spectroscopies. While these communities use their own technologies and methodologies, they share a common scientific goal of understanding the ultrafast dynamics of molecular systems or assemblies with atomic resolution. This conference was expected to strengthen bridges among these communities and foster the exchange of information and expertise.

In ICUSD 2019, the following ten topical sessions were organized: formation and dissociation of chemical bonds in metal complexes; coherent dynamics in liquid phase and related topics; ultrafast structural response of biomolecules; structural dynamics of biomolecules; conical intersection dynamics and related nonadiabatic phenomena; nonequilibrium dynamics simulation; spin crossover and strongly correlated systems; phonon and lattice-directed dynamics; structural dynamics in nanomaterials; and charge transfer and vibrational energy transfer and related structural dynamics. The conference had 151 registered participants, 29 invited speakers, 48 talks, and 85 posters from 15 countries, 58 institutes, and 78 research groups. Nine research groups kindly agreed to contribute to this special issue. Fortunately, the nine papers covered most of the topics and fields presented in the conference although some of the important ones are missing, for example, time-resolved serial crystallography, time-resolved electron/x-ray imaging, and time-resolved electron/x-ray microscopy.

As a guideline for the readers of all those fascinating papers, here I present brief comments on each of them on the order of appearance in the collection. Mizutani and co-workers measured time-resolved resonance Raman spectra to answer the question on the effect of the bound anion on the structure and dynamics of halorhodopsin in the early stage of the photocycle.[1] Chergui and co-workers monitored the structural change upon the ligand exchange of an octahedral aqueous cobalt complex using time-resolved x-ray absorption spectroscopy coupled with temperature jump via near-IR laser excitation of solvent water molecules.[2] Kim and co-workers used femtosecond transient absorption (anisotropy) spectroscopy to uncover how the length of H-aggregates of perylene bisimide influences coherent exciton coupling dynamics, thereby proposing the possibility of improving molecular optoelectronic materials through efficient energy transfer

preceding trap states of excitons in larger aggregates.[3] Cho and co-workers unveiled the effect of deep eutectic solvents on the local environment around the heme site of cytochrome c using FTIR and coherent two-dimensional IR spectroscopy.[4] Pang and co-workers investigated excited-state intramolecular proton transfers (ESIPT) of alizarin in dimethyl sulfoxide (DMSO) using femtosecond stimulated Raman spectroscopy and proposed that the solvent vibrational modes of DMSO can be used as a sensor for ultrafast chemical reactions accompanying the structural changes and subsequent solute-solvent interactions.[5] Ihee and co-workers revealed the complicated solvent-dependent photochemical reaction pathways of bromoform using both time-resolved x-ray liquidography (solution scattering) and time-resolved x-ray transient absorption spectroscopy for a wide time range from picoseconds to microseconds.[6] Cao and co-workers used time-resolved reflection high energy electron diffraction to study the thermal transport phenomena across a GaAs/AlGaAs interface heterostructure by directly monitoring the lattice temperature evolution in the time domain.[7] Weber and co-workers provided a useful comparison of femtosecond x-ray diffraction and MeV ultrafast electron diffraction (UED), which are complementary to each other, for the study of structural dynamics of gas-phase molecules.[8] Jeong and co-workers proposed a feasible MeV UED technology with high brightness and a sub-10 fs temporal resolution by using an energy filter in the dispersion section of the achromatic bend.[9]

As the readers may have noticed, the papers in this special issue cover a wide range of molecular systems, such as small molecules in the gas, liquid solution, and solid phases, solid films, and protein molecules, and a variety of time-resolved techniques such as time-resolved reflection high energy electron diffraction, femtosecond x-ray diffraction, MeV ultrafast electron diffraction, time-resolved resonance Raman spectroscopy, time-resolved temperature-jump x-ray absorption spectroscopy, femtosecond transient absorption spectroscopy, two-dimensional IR spectroscopy, femtosecond stimulated Raman spectroscopy, time-resolved x-ray transient absorption spectroscopy, and time-resolved x-ray liquidography. Nevertheless, I am afraid and also hope that, when the readers access this preface, the technologies represented by the collected papers may look outdated because the technologies of the x-ray free-electron lasers, MeV UED apparatus, and related time-resolved spectroscopy/imaging/microscopy/scattering/diffraction will continue advancing, which makes the prospect of the fields represented by ICUSD even brighter.

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