Chemical crystallography at XFELs: small molecule structure determination at lightning fast speeds

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Inorganic–organic hybrid materials are highly customizable, with adaptable ligands and desirable reaction chemistry. It is often easy to design, derivatize, and synthesize new materials faster than they can be characterized. While they often readily produce powder, consisting of millions of microcrystals, 1D powder diffraction is difficult to use for structural characterization, from unit cell determination to model building and refinement. Further, large single-crystals can be difficult to grow, can be radiation sensitive, and are often highly solvated, which makes them hard to use with single-crystal X-ray diffraction and MicroED. However, we recently showed that we could deliver microcrystalline suspensions of three hybrid materials (mithrene (AgSePh), thiorene (AgSPh) and tethrene (AgTePh)) via a liquid jet to the interaction region of an X-ray free electron laser and determine their structures. Innovations in the creation of powder patterns from single-crystal spotfinding results allowed us to determine unit cells, and we indexed the individual sparse patterns using a graph theory method that can determine crystal orientation from as few as 3 reflections. From there, we could use standard tools to solve the structures using direct methods. We will present the hardware and software challenges we overcame, show how the new structures helped us identify why thiorene is colorless, discuss how chemical SFX can help material scientists in the future to rapidly determine structures from new materials, and discuss what challenges remain for future work.