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Editorial

Time-Resolved Crystallography

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This Special Issue on 'Time-Resolved Crystallography' is a collection of eight original articles providing interesting results that give insight into the processes involved in generating and analysing time-resolved data. It includes data relevant to climate change, biological systems, and fundamentals of sample delivery and new analysis methods.

Time-resolved crystallography allows the study of intermediate states during reactions. It can provide valuable insight into the study of mechanisms at the molecular level, allowing for the identification of transition states of reactions which include catalysis, electron transfer, ligand-binding, protein interactions, and protein unfolding. It is a powerful technique that transfers "static" crystallographic structures to molecular movies, providing a better understanding of their molecular function. This Special Issue provides a space for scientists involved in this area to develop their methods and present their findings in a wide variety of areas.

The main purpose of this Special Issue is to present research which includes developing and understanding methods and processes. These articles cover a broad range of results ranging from growth studies of heterogenous ice, to the behaviour of capillary jets used in time-resolved crystallography experiments. Research scientists working in a wide range of disciplines have contributed to this Special Edition to help showcase the range of studies currently being undertaken in this field.

In this Special Issue, several topics are covered. Climate change is an important issue today. Esmaildosst et al. [1] provide insight into the understanding of how ice nucleates and grows into larger crystals in micron-sized droplets. This provides insight into the supercooling effect of clouds in our climate system. Time-resolved structural studies of both biological systems using pump-probe experiments published by Pandey et al. [2] and the time-resolved effects on lead-containing relaxor ferroelectrics by Aoyagi et al. [3] are also covered. Radiation damage, an important aspect of serial crystallography is a topic covered by Caleman et al. [4] looking at the effect on bond breaking in molecular structures, and Kozlov et al. [5] provided a theoretical study on the molecular dynamic effects at femtosecond time scales.

Sample delivery methods and characterisation is also an evolving area in this field. This topic is covered in the characterisation of capillary jet streams used in serial femtosecond crystallography experiments provided by Gañán-Calvo et al. [6], while Hadian-Jazi et al. [7] provide an analysis of how crystals interact with the X-ray beam using high-viscosity injectors generating a multi-hit crystal scenario.

Lastly, time-resolved crystallography data analysis is always evolving. Here, Adams et al. [8] demonstrate how a correlation-based technique, Pair-Angle Distribution function, can be used to extract more information form serial crystallography experiments potentially providing more information on nanoscale dynamical processes.

Conflicts of Interest: The author declares no conflict of interest.

References

1. Esmaeildoost, N.; Jönsson, O.; McQueen, T.A.; Ladd-Parada, M.; Laksmono, H.; Loh, N.-T.D.; Sellberg, J.A. Heterogeneous Ice Growth in Micron-Sized Water Droplets Due to Spontaneous Freezing. *Crystals* **2022**, *12*, 65. [CrossRef]
2. Pandey, S.; Poudyal, I.; Malla, T.N. Pump-Probe Time-Resolved Serial Femtosecond Crystallography at X-ray Free Electron Lasers. *Crystals* **2020**, *10*, 628. [CrossRef]
3. Aoyagi, S.; Aoyagi, A.; Takeda, H.; Osawa, H.; Sumitani, K.; Imai, Y.; Kimura, S. Time-Resolved Nanobeam X-ray Diffraction of a Relaxor Ferroelectric Single Crystal under an Alternating Electric Field. *Crystals* **2021**, *11*, 1419. [CrossRef]
4. Caleman, C.; Jares Junior, F.; Grånäs, O.; Martin, A.V. A Perspective on Molecular Structure and Bond-Breaking in Radiation Damage in Serial Femtosecond Crystallography. *Crystals* **2020**, *10*, 585. [CrossRef]
5. Kozlov, A.; Martin, A.V.; Quiney, H.M. Hybrid Plasma/Molecular-Dynamics Approach for Efficient XFEL Radiation Damage Simulations. *Crystals* **2020**, *10*, 478. [CrossRef]
6. Gañán-Calvo, A.M.; Chapman, H.N.; Heymann, M.; Wiedorn, M.O.; Knoska, J.; Gañán-Riesco, B.; López-Herrera, J.M.; Cruz-Mazo, F.; Herrada, M.A.; Montanero, J.M.; et al. The Natural Breakup Length of a Steady Capillary Jet: Application to Serial Femtosecond Crystallography. *Crystals* **2021**, *11*, 990. [CrossRef]
7. Hadian-Jazi, M.; Berntsen, P.; Marman, H.; Abbey, B.; Darmanin, C. Analysis of Multi-Hit Crystals in Serial Synchrotron Crystallography Experiments Using High-Viscosity Injectors. *Crystals* **2021**, *11*, 49. [CrossRef]
8. Adams, P.L.R.; Binns, J.; Greaves, T.L.; Martin, A.V. Using the pair angle distribution function for analysing protein structure. *Acta Crystallogr. Found. Adv.* **2021**, *77*, C574. [CrossRef]