Looking for order in disorder: topological data analysis of glass structure

Invited Talk

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Looking for order in disorder: topological data analysis of glass structure

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An important question to unravel within materials science is the interplay between structure and properties in glass materials. To understand this link, there has been a great interest in pinpointing structural features that correlate strongly with the properties. However, identifying such structural descriptors especially at the medium-range length scale remains a challenging task. In this talk, we present our work on using topological data analysis to reveal hidden medium-range order (MRO) in oxide and hybrid glasses. Specifically, we apply persistent homology, a type of topological data analysis, to categorize and understand MRO structure in these systems, for which the atomic configurations have been generated by molecular dynamics simulations. By using persistent homology to study the size of certain algebraic topological features, we observe similarities to the length scales associated with the well-known first sharp diffraction peak in the studied glasses.

Reference: S.S. Sørensen, C.A.N. Biscio, M. Bauchy, L. Fajstrup, M.M. Smedskjaer, Revealing Hidden Medium-Range Order in Amorphous Materials using Topological Data Analysis, *Science Advances* **6**, eabc2320 (2020).