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Topological data analysis as a tool to analyze the structure of amorphous materials

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The medium-range order (MRO) structure of glasses and other amorphous materials impact a range of their physical and chemical properties. Nonetheless, MRO in amorphous systems remains poorly understood due to the limited experimental and computational probes. However, recent developments in persistent homology (PH), a type of topological data analysis, provide a new path for categorizing and understanding MRO structure in amorphous materials. In this talk, we will show how PH can be used to analyze the MRO structure of archetypical sodium silicate glasses, for which the atomic configurations have been generated by classical molecular dynamics simulations. By employing PH to study the size of certain algebraic topological features, we observe striking similarities to the length scales associated with the well-known first sharp diffraction peak. We also discuss how recent tools from topological data analysis can be applied to categorize and compare topological features at the atomic scale. Overall, we expect the developed methodology to be easily extendable to understand MRO in other amorphous systems, whenever the atomic configuration can be reliably obtained. Finally, we will discuss the perspectives of applying persistent homology tools within materials science in general.

Reference: Sørensen, S. S., Biscio, C. A. N., Bauchy, M., Fajstrup, L., Smedskjaer, M. M., Revealing hidden medium-range order using topological data analysis. *Science Advances* **6**, eabc2320 (2020)