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Understanding Medium-Range Order Structure of Glasses using Persistent Homology

Søren S. Sørensen¹, Christophe A. N. Biscio², Mathieu Bauchy³, Lisbeth Fajstrup², Morten M. Smedskjaer¹

¹*Department of Chemistry and Bioscience, Aalborg University, Denmark*

²*Department of Mathematical Sciences, Aalborg University, Denmark*

³*Department of Civil and Environmental Engineering, University of California, Los Angeles, USA*

The medium-range order (MRO) structure of glasses can significantly influence their properties, yet the understanding of MRO, particularly in relation to the origin of the first sharp diffraction peak (FSDP) in the structure factor, remains elusive. Recent developments in persistent homology (PH), a type of topological data analysis, provide a new path for analyzing MRO structure in amorphous materials. In this work, we employ PH to analyze the MRO structure of sodium silicate glasses, which in turn has been obtained by classical molecular dynamics simulations. By studying the size of certain topological features, we find striking similarities to the length scales associated with the FSDP. In addition, we find that PH captures the compositional dependence of the FSDP in the sodium silicates. Overall, we expect the developed methodology to be easily extendable to understand MRO in other glassy systems, whenever the atomic positions can be reliably obtained.

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