



AALBORG UNIVERSITY
DENMARK

Aalborg Universitet

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

Invited Talk

Smedskjær, Morten Mattrup; Sørensen, Søren Strandkov; Biscio, Christophe; Fajstrup, Lisbeth; Bauchy, Mathieu

Publication date:
2021

[Link to publication from Aalborg University](#)

Citation for published version (APA):

Smedskjær, M. M., Sørensen, S. S., Biscio, C., Fajstrup, L., & Bauchy, M. (2021). *Looking for order in disorder: topological data analysis of glass structure: Invited Talk*. Abstract from Materials Science & Technology 2021, Columbus, Ohio, United States.

General rights

Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

- Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
- You may not further distribute the material or use it for any profit-making activity or commercial gain
- You may freely distribute the URL identifying the publication in the public portal -

Take down policy

If you believe that this document breaches copyright please contact us at vbn@aub.aau.dk providing details, and we will remove access to the work immediately and investigate your claim.

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

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

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

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).