Research Title Description and feature extraction of amorphous structure based on topological data analysis

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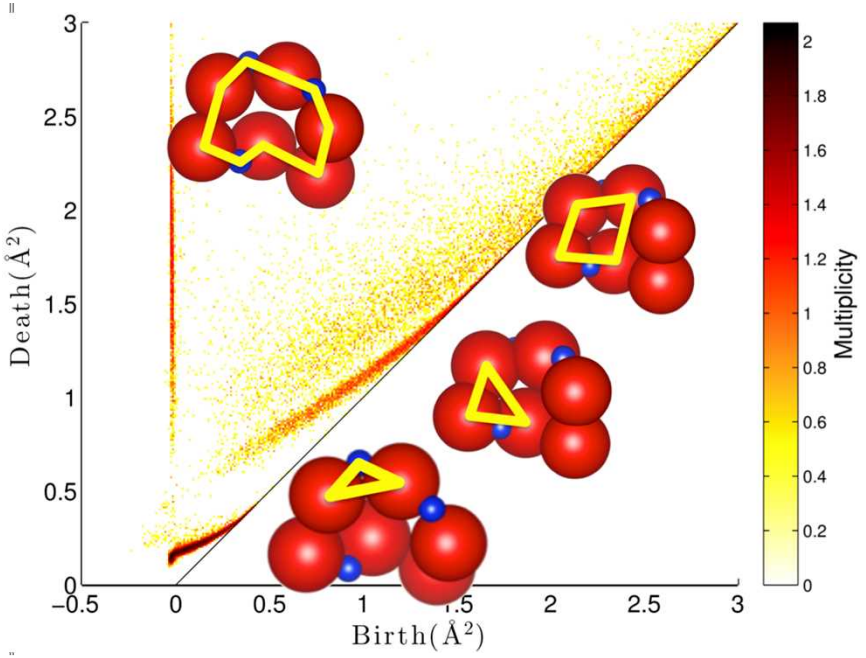
Research Area : Advanced Materials Informatics through Comprehensive Integration among Theoretical, Experimental, Computational and Data-Centric Sciences（PO：Shinji Tsuneyuki）

Brief overview

1.Based on Topological Data Analysis (TDA), we have constructed a framework to describe the microscopic structure, in particular the disordered structures that are unfavorable in traditional material sciences
2.We have constructed the theory and calculation method of free energy landscape independent of variable selection based on differential geometry and stochastic process.
3.We have developed the connection between the structural feature expressed by TDA and materials property through free energy landscape calculation.

Achievement

1.Based on TDA, we have constructed an expression reflecting the hidden structure embedded in a disordered structure. Focusing on two examples: silica glass as a random continuous network former and metallic glass as a forming a random packed structure, we have proposed a unified the expression of these structure which was expressed in different methods.
2.Data-driven methods, typically TDA, often use variable of structural feature without physical interpretation. Our new definition of free energy landscape is free from the interpretation.
3.By combining the achievements, we are now able to introduce statistical physics techniques to TDA.



Description of Microscopic Structure Based on TDA

Reference/Link

1 https://doi.org/10.1073/pnas.1520877113
2 https://arxiv.org/abs/1803.09034