

TOPOLOGICAL DATA ANALYSIS ON AMORPHOUS STRUCTURES

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Description of amorphous structures has been a long standing problem. What is lacking there is an appropriate language to describe geometric structures including short-range order (SRO) and medium-range order (MRO). In this talk, we present computational topological methods based on persistent homology and apply them into atomic arrangements of silica (SiO_2) and granular systems. The results elucidate the following new geometric features in amorphous structures: (i) clear identification of amorphous states in silica by using persistence diagrams, (ii) hierarchical relationships between SRO and MRO in silica, (iii) presence of specific packing states (FCC, HCP, BCC, etc) in three dimensional granular packing experiments and transitions among them.