Persistent Homology and Optimal Transport to Characterize Chemical Reactivity in Dynamic Systems

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Abstract: As a computational tool, persistent homology identifies topological features of a space at different filtration levels. For point cloud data, monitoring the connected components as a function distance allows for compact barcode representations of the spatial organization or configuration of a chemical system. Using concepts of optimal transport, one can then consider distance metrics (i.e., Wasserstein distance) between barcode distributions as a means to characterize differences in geometric organization of atoms or molecules. In dynamic systems, analysis of the fluctuations in barcode representation and associated Fourier transforms can be used to identify chemical reactivity as recently reported in DOI: 10.3389/fchem.2021.624937. Extension and adaption of this concept is now being used to study electron density evolution during chemical reactions as will be described in this presentation.