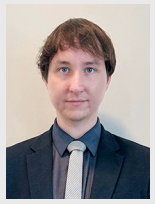
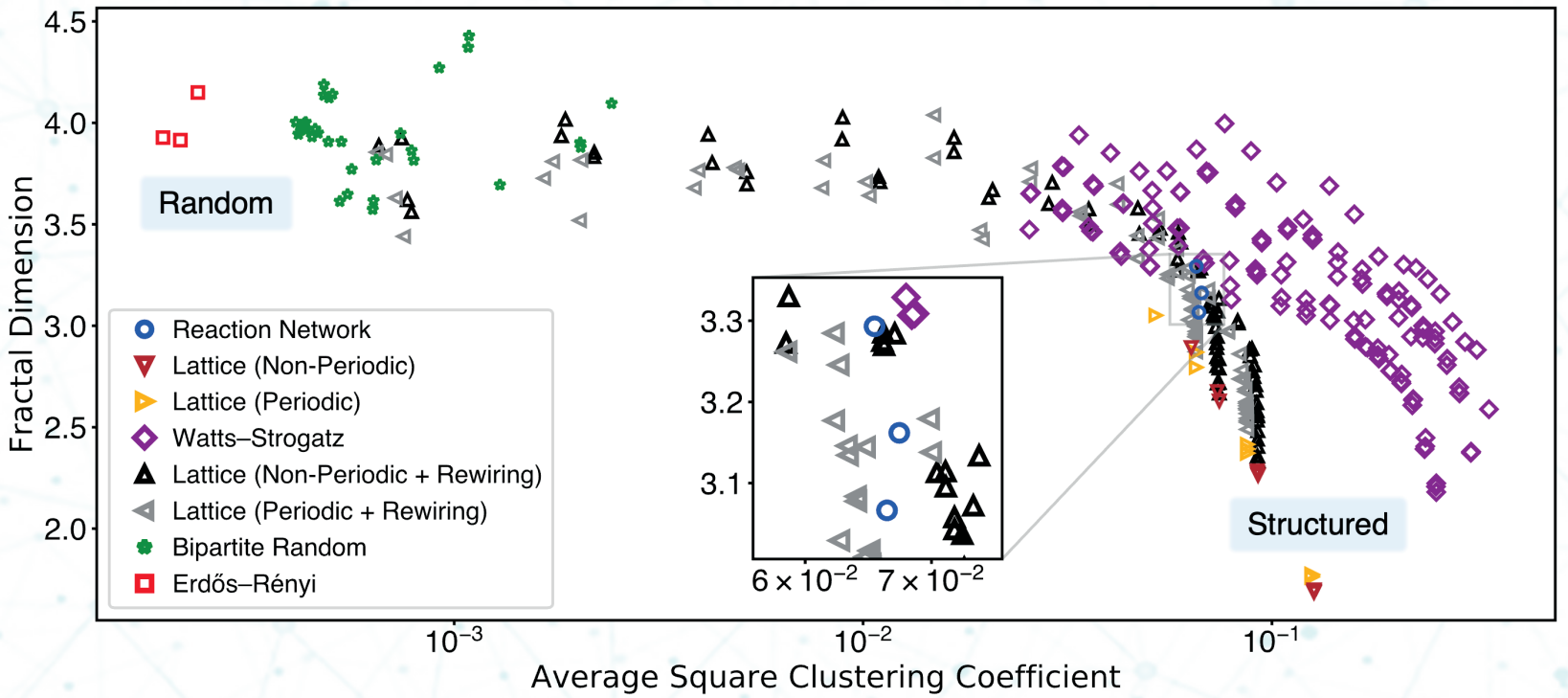
Reaction Networks Resemble Low-Dimensional Regular Lattices



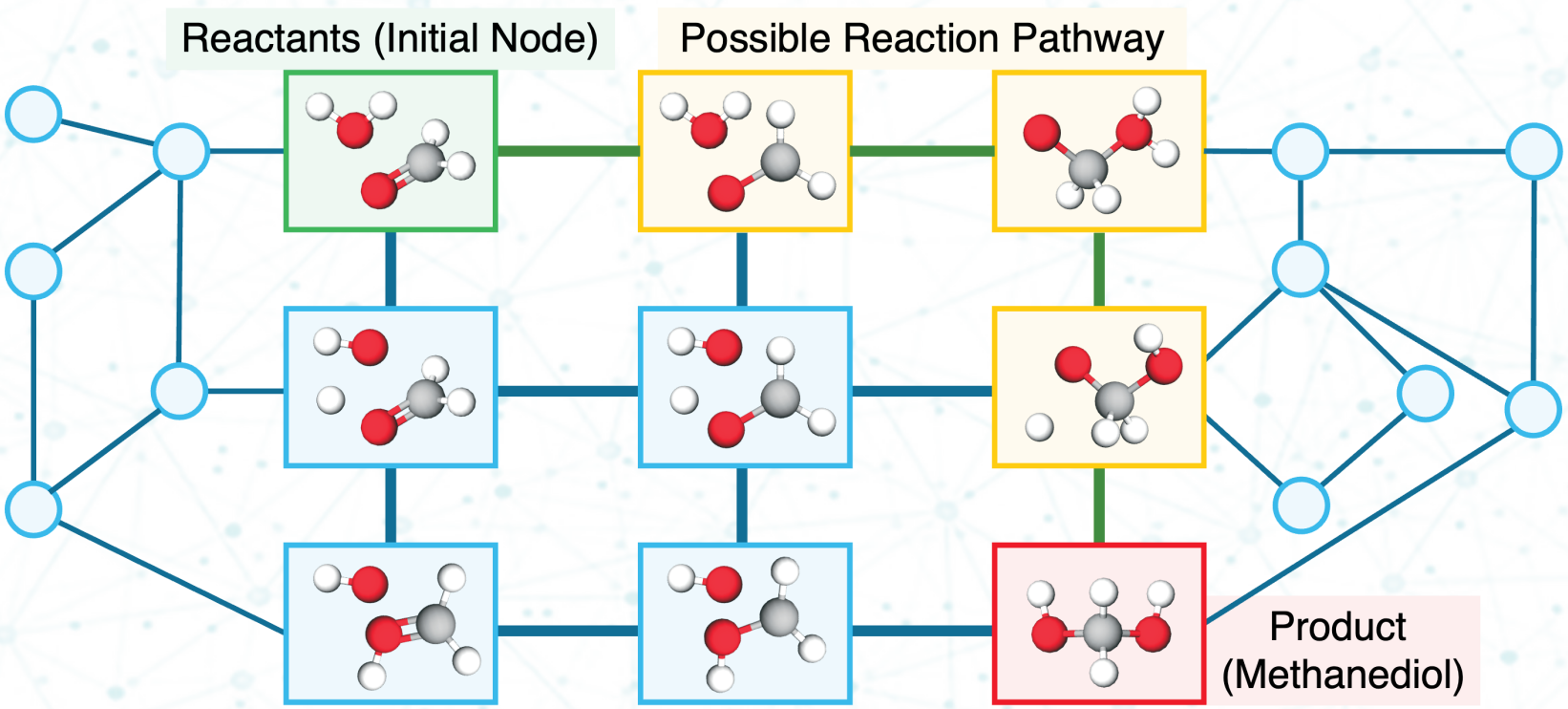
Exploring the vast and diverse chemical space of possible molecular structures is key to discovering new molecules and predicting reactions pathways. However, its dimensionality grows exponentially with each additional atom, making exploration challenging. To enable the exploration of chemical space, we developed a lower-dimensional discrete reaction network representation, where nodes are collections of molecules with fixed stoichiometry (number of atoms) and edges are stoichiometry-preserving transformation rules, i.e., bond breaks and bond formations. To understand the inherent structure of reaction networks, which are expensive to generate, we compared reaction networks composed of Carbon, Hydrogen, Nitrogen, and Oxygen against various known generative network models. Our comparison encompasses networks constructed randomly, such as Erdős–Rényi networks, networks constructed following a regular pattern such as a regular lattice, and networks constructed following a regular pattern with an adjustable probability to rewire connections, such as Watts-Strogatz networks. Examining fundamental network properties, such as the fractal dimension and the average square clustering coefficient, revealed that reaction networks closely resemble low-dimensional regular lattices with intermittent random rewiring of edges. This insight is important as it suggests that we can explore these networks more effectively by leveraging their regular structure.

Miko Stulajter *and Dmitrij Rappoport*

This research is supported by the National Science Foundation grants (CHE-2227112 and DUE-1930546) and the Computational Science Research Center (CSRC) at San Diego State University



Plot of fractal dimension versus average square clustering coefficient, comparing reaction networks (circles) with various generative models: Watts-Strogatz networks (diamonds), regular lattices with dimensionality, $d = 2–5$, with non-periodic boundary conditions (down triangles) and periodic boundary conditions (right-facing triangles), along with rewired versions (up triangles and left-facing triangles, respectively), bipartite random networks (stars), and Erdős–Rényi networks (squares). Reaction networks are more structured and most similar to lattices with a small amount of rewiring.



Reaction network for two oxygen, one carbon, and four hydrogen atoms, starting with formaldehyde (CH_2O) and water (H_2O) as the initial reactants. The lattice-like structure of reaction networks can be seen clearly in the network. The highlighted path (orange nodes) traces the transformation from the reactants (green node) to the product, methanediol ($CH_2(OH)_2$) (red node). Molecular diagrams along the path depict the specific bonds broken and formed at each step.