Descriptors of Energy Landscapes using Topological Analysis

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DELTA NSF #1934725
Descriptors of Energy Landscapes Using Topological Analysis

3N Energy Landscape (Simulation/Experiment) → Dimensionality Reduction → Topology of Reduced Energy Landscapes → Predictive Machine Learning → Accelerated Sampling

- PCA
- Non-linear Methods
- Generalized Collective Coordinates
- Morse Theory
- Persistent Homology
- Catastrophe Theory
- Singularity Theory

Optimized Synthetic Conditions
Phase Behavior
Tuning Catalytic Pathways

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• While a merge tree summarizes the connected components in an energy landscape, it does not portray the shape of each connected component.
• The two energy landscapes in (a) and (b) have the same merge tree (c).
• Nevertheless, the connected components in (a) are always contractible, whereas those in (b) may contain holes, as shown by the sublevelset in (d).
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• Nevertheless, the connected components in (a) are always contractible, whereas those in (b) may contain holes, as shown by the sublevelset in (d).
Persistent Homology and Machine Learning

• Goal: Learn to identify and leverage changing topological features of energy landscapes across a range of chemical conditions in order to predict reactivity.

• Persistent homology makes topology **quantitative**, and there are a suite of tools (persistence landscapes, persistence images) for incorporating topological features into machine learning algorithms.
Homology

The $i$-dimensional homology group
Input: Real-valued function on a space. Output: barcode.
Sublevelset persistent homology of the $n$-alkanes
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Sublevelset persistent homology of pentane

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Sublevelset persistent homology of the $n$-alkanes

- We have a formula for the birth and death time of each bar in every homological dimension

- The proof uses a Künneth formula for persistent homology by Jose Perea and Hitesh Gakhhar

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A notion of distance between energy landscapes

Bottleneck and Wasserstein distances are “edit” distances between barcodes
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Odd-even effect in liquid \( n \)-alkanes

**Figure 1.** a) Melting points and boiling points of \( n \)-alkanes \((n = 5–10)\) as a function of their backbone length \( n \). b) Density and viscosity of \( n \)-alkanes near their respective melting points \((T_m + 3 \text{ K})\). Error bars herein represent one standard deviation.

*Dynamic odd-even effect in liquid \( n \)-alkanes near their melting points* by Ke Yang, Zhikun Cai, Abhishek Jaiswal, Madhusudan Tyagi, Jeffrey S Moore, Yang Zang.
Odd-even effect in liquid n-alkanes

Figure adapted from: R. Boese et al. Angew. Chem. Int. Ed. 1999, 38(7)

Figure adapted from: K. Yang et al. Angew. Chem. Int. Ed. 2016, 55, 14090-14095
Machine learning tasks

• Big goal: Predict how the energy landscape of a chemical system evolves as a result to changes in salinity, temperature, pressure, etc.

• Related subgoal: Predict how the sublevelset persistent homology evolves as a result to changes in salinity, temperature pressure, etc.
  • Halide task

\[
\begin{align*}
&H & H & H & H & H \\
H & C & C & C & C & C & H \\
H & H & H & H & H & \text{Br}
\end{align*}
\]
Molecular dynamics simulation samples the EL

Numerical, $k_B T = 16.6$ (kJ/mol)

Analytical
Point-cloud data
Cyclo-Octane

Topology of cyclo-octane energy landscape
Martin, Thompson, Coutsias, Watson, 2010
Cyclo-Octane

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