Representations of Energy Landscapes by Sublevelset Persistent Homology: An Example with n-alkanes

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Descriptors of Energy Landscapes Using Topological Analysis

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

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

Phase Behavior → Tuning Catalytic Pathways

Energy

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COLLECTIONS

Note: This paper is part of the JCP Special Collection in Honor of Women in Chemical Physics and Physical Chemistry.

This paper was selected as an Editor’s Pick
Merge trees and sublevelset persistent homology
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- Local minima
- index 1 saddle that merges two components
- index 1 saddle that creates a loop
- Index 2 critical point

Merge tree

0-dim persistent homology

1-dim persistent homology
Butane

Pentane

Hexane

Energy \( f: S^1 \to \mathbb{R} \)

Energy \( f(\phi_1) + f(\phi_2) \)

Energy \( f(\phi_1) + f(\phi_2) + f(\phi_3) \)
Sublevelset persistent homology of pentane (OPLS-UA)
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We have a complete characterization of the sublevelset persistent homology of all alkanes \( f : (S^1)^n \to \mathbb{R} \).

# bars is \( \frac{(6^n + 2^n)}{2} \)

# bars in dimension \( k \) is \( \binom{n}{k} + (3^k - 1)(\binom{n-1}{k}) \)
The proof of how the birth and death times pair uses "Kümeth formulae in persistent homology" by Hitesh Gakhar and Jose Perea.
A notion of distance between energy landscapes.

Bottleneck and Wasserstein distances are "edit" distances between barcodes.
Molecular dynamics simulation samples the EL

Numerical, $k_B T = 16.6 \text{ (kJ/mol)}$

Analytical
Ongoing and future work

(DELTA, Aurora Clark, Biswajit Sadhu, Brittany Story, Ethan Berkove, Jose Perey)

• Branched alkanes - any tree!

• Alkenes and alkynes

• Cyclo-alkanes

• Machine learning

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