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Johnathan Bush* (bush.j@ufl.edu). *Sublevelset persistent homology of the n -alkane potential energy landscapes.*

The graph of a real-valued function defined on the set of configurations of a molecule is an example of an energy landscape. Disconnectivity graphs, which summarize the connectivity of the local minima of an energy landscape via the lowest-barrier pathways, are a common representation of complex and high-dimensional regions of an energy landscape. However, there is more information to be gained by also considering the topology of each connected component at different energy thresholds (or sublevelsets). We consider the straight-chain alkanes as a motivating example and derive a formula for the sublevelset persistent homology of the potential energy landscapes of these molecules in all homological dimensions.

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