1163-55-189 **Henry Adams*** (henry.adams@colostate.edu), Colorado State University, Department of Mathematics, Fort Collins, CO 80523. *Descriptors of Energy Landscapes using Topological Analysis (DELTA).*

Many of the properties of a chemical system are described by its energy landscape, a real-valued function defined on a high-dimensional domain. I will explain how topology, and in particular persistent homology, can be used in order to describe some of the pertinent features of an energy landscape. Whereas a merge tree encodes how connected components of an energy landscape evolve as the energy level increases, persistent homology can also quantify the shape of these connected components. As a motivating example, we completely describe the sublevelset persistent homology of the n-alkanes. Our proof of the number of sublevelset persistent homology bars is completely combinatorial; indeed we proceed by induction on the number of carbons in the alkane chain. Our proof of the lengths of the bars is more topological, relying on the Künneth formula. In a recently funded NSF Harnessing the Data Revolution project, the DELTA team is learning how to identify and leverage changing topological features of energy landscapes across a range of chemical conditions in order to predict reactivity. (Received August 25, 2020)