

Representation of Reaction Networks by Generative Topographic Mapping

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Ab initio kinetic studies provide a microscopic insight into reaction mechanism by exploring reaction paths. Traditionally, a reaction network is represented by a connected graph in which the nodes represent stationary 3D structures whereas edges correspond to chemical transformations. However, the visualization and analysis of a network containing thousands of nodes is challenging. Alternatively, we propose to use for this purpose the Generative Topographic Mapping (GTM), a probabilistic dimensionality reduction method.

A reaction network for ethylene hydrogenation with a transition metal complex inspired by Wilkinson's catalyst was obtained with the help of the Artificial Force Induced Reaction (AFIR) method. A serie of GTMs, each accommodating about a million of geometries, identifies the areas of high and low energy, some zones populated by physically irrelevant 3D structures and those corresponding to different steps of the reaction path. The expansion of the reaction chemical space in course of DFT calculations was monitored by successive projections on the GTM manifold.