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Computationally Efficient Characterization of Potential Energy Surfaces Based on Fingerprint Distances[1] BASTIAN SCHAEFER, STEFAN GOEDECKER, University of Basel, GOEDECKER GROUP TEAM — Based on Lennard-Jones, Silicon, Sodium-Chloride and Gold clusters, it was found that uphill barrier energies of transition states between directly connected minima tend to increase with increasing structural differences of the two minima. Based on this insight it also turned out that post-processing minima hopping data at a negligible computational cost allows to obtain qualitative topological information on potential energy surfaces that can be stored in so called qualitative connectivity databases. These qualitative connectivity databases are used for generating fingerprint disconnectivity graphs that allow to obtain a first qualitative idea on thermodynamic and kinetic properties of a system of interest.

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Bastian Schaefer
University of Basel

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