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Exploring Topographies and Dynamics on Many-Dimensional Landscapes

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A major challenge to understanding and using kinetics is finding the relationships between the topography of the many-dimensional potential energy landscape (or landscapes, for systems with multiple accessible electronic states) and the way that topography, local and large-scale, determines how systems change their structures, relax and anneal. One major difficulty is simply the complexity of the landscape; one is forced to work with small statistical samples of the surface; how should these samples best be chosen? What characteristics of the topography provide the most important information? Another: how does the nature of the interparticle forces determine the topography and hence the character of motion on the surface? And what are the most useful diagnostic tools to tell us about that behavior? We shall address these questions, more in terms of progress toward, rather than providing definitive answers.