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Characterizing the potential energy landscape by its geodesic paths CHENGJU WANG, RICHARD M. STRATT, Department of Chemistry, Brown University, Providence, RI 02912 — We suggest that the time evolution of a condensed-matter system is related to a unique exploration path in its multidimensional potential energy surface. We show that sampling from what we call the potential energy landscape filling ensemble, we can study the potential energy landscape of a monatomic Lennard-Jones system without the complications of barrier hopping processes. The ensemble defined to include all the configurations with potential energy less than a specified value, allows us to sample the geodesic path between two randomly selected configurations. The geodesics were tentatively related to the dynamics of the system under the assumption that the geodesic path corresponds to the most efficient exploration route on its potential energy surface. The derived dynamic parameters were compared with those obtained from a molecular dynamics simulation. The agreement we found offers us a new method for relating the dynamics of a system to the topology of its static potential energy surface.

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