Energy landscapes in chemistry - from solids to molecules and surfaces

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In many areas of science, problems are frequently encountered which exhibit an underlying complex multi-minima energy landscape. Examples range from aging in physical and chemical systems to metastable chemical compounds and glassy systems, and optimal control of e.g. crystal growth, just to name a few instances. To address these questions and deal with the time evolution of such systems, it is necessary to develop new general concepts for analyzing such landscapes and suitable global exploration algorithms to obtain global and local information about the structure of the energy landscape.

In this talk, I am going to give an introduction to basic landscape concepts such a local ergodicity[1,2,3] and generalized barriers[4,2], together with presenting algorithms that go beyond standard global optimization techniques[2]. These are illustrated by a number of examples drawn from chemistry, including the structure prediction via global exploration of energy landscapes of chemical systems such as crystals[3,5,6], molecules[2], clusters[7], monolayers[8], molecules on surfaces[9], growth of films in chemical synthesis[10], and aging in amorphous ceramics[11].

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