# Structure prediction in nanomaterials

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The drive to develop new materials with well-specified properties lies behind the creation of a new class of materials, the so-called nanomaterials. They bridge the gap between classical multi-crystalline, crystalline and amorphous materials, and individual molecules and clusters of various sizes. The combination of small size with (partly) regular extended structure and a relatively large surface-to-volume ratio leads to the existence of many modifications of a nano-object for the same overall composition. This structural plethora allows us to tune the physical and chemical properties of the nanomaterial to a much larger degree than possible in macroscopic materials.

On the other hand, it is considerably more difficult to analyze the atomic arrangements of these nano-particles, and thus theoretical tools are needed to determine or even predict the (possible) structures present in the chemical system. Both the investigation of the wide range of possible structures in the system and the analysis of their stability require the study of the energy landscape of the system: the determination of the minima on the landscape and the generalized barriers separating them. Furthermore, the possible design of nanomaterials, e.g. via atom by atom or atom cluster by atom cluster assembly, or via the controlled deposition of molecules on surfaces, relies on information about the properties of the corresponding energy landscape.

In this presentation, we introduce the basic concepts of energy landscapes, and show applications of energy landscapes to crystalline compounds and nanomaterials. Examples of crystalline compounds will include the successful prediction of (by now synthesized) compounds, such as LiBr[1,2] and LiCl[1,3], and of (by now achieved) high-pressure phases, such as $Rb_2S$[4,5] and $Cs_2S$[4,6], and the interaction between theory and experiment in the exploration of the phase diagram of (Li,Cs)Cl[7]. With regard to nanomaterials, we will present the theoretical analysis[8] of a newly synthesized[9] phase of few-layer MgO films on an $Al_2O_3$ substrate, which we suggest to exhibit the 5-5 structure that had been predicted in earlier work to be metastable for MgO[10]. More examples of structure prediction in nanomaterials (clusters, two-dimensional systems, molecules on surfaces, etc.) can be found in refs. [8,11].

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