Overview of modern computational methods in the research of advanced materials from bulk crystals to nanoscale structures

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In the first part of this overview we present crystal structure prediction using simulated annealing in the lead sulfide [1] and zinc oxide [2] compound, calculated using empirical potentials and on the *ab initio* level. The results were in good agreement with previous theoretical and experimental observations, and we have found some additional structure candidates as function of pressure. Next, we show results for an *ab initio* minimization data mining approach, which combines two computational methods. In this study we have investigated binary materials with elements from groups V, IV - VI, and III – VII, with the goal to identify chemical systems where recently proposed "5-5" crystal structure type might be experimentally accessible and, among others, TlF, SnO, SnS, SnSe, GeS, GeSe, PbO, PbS, ZnO and ZnS, were chosen for the study [3]. In the third part of this overview, we show calculations performed in the ZnO system using the prescribed path algorithm, where we have investigated the connectivity among experimental ZnO crystal structures on the energy landscape, and in particular transition states [4]. With the results of this study we were able to understand more about the influence of temperature in ZnO, to connect our results to the actual synthesis routes and get additional crystal and nanostructured candidates.

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