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Simulations of structural phase transitions in crystals by metadynamics

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Abstract: Crystal structure prediction problem is an important problem in physics, chemistry and materials science. Besides methods based on stochastic generation of candidate structures a possible approach is to study structural phase transitions between different polymorphs. In addition to information about new structures the latter approach provides also useful hints to microscopic mechanisms of structural transitions on atomistic level which are difficult to extract from experiments. Computer simulations of structural transformations in crystals, however, present a non-trivial problem due to high barriers separating different crystalline phases. The talk will present an overview of basic principles and some applications of the metadynamics-based algorithm for simulation of structural phase transitions in crystals [1,2,3,4]. The approach is based on the general metadynamics algorithm [5] and uses the supercell matrix as collective variable driving the system from one crystal structure to another, following low free-energy pathways. By effectively introducing a mechanism allowing crossing of barriers it eliminates the need for substantial overpressurization typically needed in constant-pressure MD simulations, resulting in more realistic transformation mechanisms as well as substantially improved predictive power. It also enables simulation of complex reconstructive transitions with transformation pathways proceeding via several intermediate states. The algorithm has been successfully applied to study of high-pressure structural transformations in various materials, such as MgSiO3 (post-perovskite phase) [6], SiO2 [7], Si [8], CO2 [9], C [10], Ca [11], BN [12] etc.

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