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Predicting crystal strucutres by metadynamics

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Recently we introduced a new method for the study of structural transformations in crystals [R. Martonak, A. Laio and M. Parrinello, Phys. Rev. Lett., 90, 075503 (2003)] which represents a conceptual extension of the idea of constant-pressure simulation. Instead of the latter, we start from the initial crystal structure and perform a search for new minima of the Gibbs potential, corresponding to new structures. The exploration of the free energy surface is performed in the space of the parameters of the simulation cell (as in Parrinello-Rahman) by means of a coarse-grained dynamics (metadynamics) [A. Laio and M. Parrinello, PNAS, 99, 12562 (2002)]. We illustrate the power of the method by studying the pressure-induced structural transition in a model of silicon. We also discuss recent results obtained by applying the method to structure prediction in zeolites and organic crystals (benzene), showing that even in complex polyatomic materials our approach allows an efficient prediction of the polymorphs.