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Mechanism of Polymorphic Transformations in the Chemical Elements

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The prediction of a crystal structure at given composition and thermodynamic coupling parameters is a major challenge. Powerful methods have boosted progress in this field, recently, and have promoted this are of research into a multidisciplinary one. The capacity of anticipating the outcome of a synthetic effort, or the search for novel materials with distinct, improved properties greatly benefit from numerical methods able to efficiently scan for novel structural motifs. Several techniques based on evolutionary algorithms, metadynamics, random structure prediction, or transition path sampling are contributing important advances in the understanding of polymorphic transformation, and are enriching the catalogue of crystalline matter by surprising novel packings [1]. One of the central aspects to fully unfold the impact of crystal structure prediction is the elucidation of transformation mechanisms, which are productive towards a particular structural motif under experiment-relavant conditions. In the recent dispute on the structural identity of the product of graphite cold compression, the true product was confirmed to be Oganov's M-Carbon by applying transition path sampling [2]. While many carbon polymorphs can exist in principle, kinetic control will typically select a particular mechanism of formation of a distinct carbon. This proves that, while the enumeration of crystal structures is invaluable in discovering novel material with improved properties, and in exploring novel compositions, it is important to associate a mechanism with the formation of a particular structure, for a realistic crystal structure prediction, one that can be turned into a real material. The talk will have a review character, and will touch upon recent results in the filed of the polymorphism of the elements and binary semiconductors [3].

[1] *Oganov, A. R. Modern Methods of Crystal Structure Prediction (Wiley-VCH, 2011),* ***[2]*** *S. E. Boulfelfel, A. Oganov, S. Leoni, Scientific Reports 2, 471, 2012.,* ***[3]*** *D. Selli, I. Baburin, R. Martoňák, S. Leoni, Phys. Rev. B 84, 161411 (2011)*

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