**Crystal Structure Prediction: Theory, Applications and Challenges**

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Although crystal structure prediction from first principles is now less controversial and more mainstream than when the first applications were reported in the early 1990's, it is debatable whether it is possible to reliably predict the observable polymorphs of simple organic molecules.

In this contribution, the theory of crystal structure prediction will be reviewed and illustrated with recent application examples (e.g., [1, 2]), including the three so-called 'blind tests' organised by the Cambridge Crystallographic Data Centre [3].

Despite significant progress since the early 1990's, many challenges still remain, such as the treatment of flexible molecules and the accurate description of polymorphic stability [4]. Related areas of research that merit particular attention are the simulation of crystal nucleation and the consideration of kinetics in crystal growth simulations [5]. The latest research aims to address the fundamental question why certain polymorphs crystallise and grow, whereas other structures, which are predicted to be thermodynamically stable, cannot be obtained experimentally.

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**Keywords: polymorphism, crystal modelling, molecular mechanics**