

**MS14 O1**

**The blind tests of crystal structure prediction. 15 years of development: where are we now?** Graeme M. Day,  
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**Keywords: crystal structure prediction, molecular crystals, computer simulation**

The ambitious goal of predicting the crystal structure of a molecule, given only a molecular diagram, is a great challenge for the molecular modelling community. The problem has led to the development of a variety of methods, both for sampling the space of all possible close-packed crystal structures and for assessing the most likely structure(s) from the subsequent list of possibilities.

Blind tests of crystal structure prediction have been organised by the Cambridge Crystallographic Data Centre as an objective evaluation of existing methodologies. For these challenges, molecules were chosen whose crystal structures were previously unknown. Their crystal structures were determined and withheld by an independent referee for the duration of the test. Diagrams of the molecules were presented to the community and participants asked to submit their three most likely crystal structures for each; these predictions were then compared to the experimentally determined structures.

Previous blind tests [1] have highlighted the main challenges in crystal structure prediction. For example, there has only been one successful prediction for a conformationally flexible molecule in all three earlier challenges. Some results from the recently completed fourth blind test are presented here, in the context of previous blind tests and recent advances in methodologies.

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**MS14 O2**

**Molecular structure and properties: Looking at hydrogen bonds.** Enrique Espinosa<sup>a</sup>, Ignasi Mata<sup>b</sup>, Ibon Alkorta<sup>c</sup>, Elies Molins<sup>b</sup>, <sup>a</sup>*LCM3B, University Henri-Poincaré, Nancy, France.* <sup>b</sup>*ICMAB-CSIC, Barcelona, Spain.* <sup>c</sup>*IQM-CSIC, Madrid, Spain.*  
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Molecular structure is determined by nuclei positions. From the Hellmann-Feynman theorem [1] we know that the exact ground state electron density distribution  $\rho(\mathbf{r})$  depends on the nuclei positions only. Furthermore, the Hohenberg-Kohn theorem [2] states that the total energy of a system can be written in terms of this distribution. In that context, the relationship between the structure of a molecular system and its physical and chemical properties, in particular energetics, should be reflected by the electron distribution. Accordingly, hydrogen bonding interactions described in terms of the electron density distribution can be considered as a fundamental subject of study to get insight on their structure-properties relationship, as the former,  $\rho(\mathbf{r})$ , is a conceptual bridge between the latter. On the other hand, the topological analysis of  $\rho(\mathbf{r})$  developed by Bader and co-workers [3] is a very useful tool for

characterizing atomic interactions in internuclear regions. Thus, within this framework, the structure-properties relationship of hydrogen bonds will be discussed in terms of the topological analysis of experimental and theoretically calculated electron density distributions that have been characterized in hydrogen bonding regions [4-9].

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**MS14 O3**

**Crystal structures of moderately complex organic molecules are predictable** Marcus A. Neumann, *Avant-garde Materials Simulation, 30 bis rue du vieil Abreuveoir, 78100 St-Germain-en-Laye, France.*

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**Keywords: crystal structure prediction, lattice energy ranking, force field parameterization**

A comprehensive computational strategy for the prediction of crystal structures with an unprecedented success rate is presented. Key components are a hybrid method [1] for the accurate calculation of lattice energies, a robust procedure for the parameterization of tailor-made force fields and a novel approach for crystal structure generation. The hybrid method combines DFT calculations by means of the VASP program [2-4] with an empirical van der Waals correction. It is used for the final lattice energy ranking and acts as a reference standard for force field parameterization. A tailor-made force field is derived for each molecule for which the crystal structure is to be predicted. The apparently simple force field involves bond increments, isotropic van der Waals potentials and essentially uncoupled intramolecular energy terms, but the mathematical framework of the force field and the fitting procedure have been designed to allow for a maximum amount of customizability while avoiding redundancy. Hundreds of force field parameters can be optimized simultaneously and typical disagreements between the tailor-made force field and the hybrid method lie in the range of 0.015-0.03 kcal/mol per atom. The tailor-made force field is used for crystal structure generation and for the preparation of Hessian matrices for the final lattice energy optimization with the hybrid method. Based on the known statistical deviation between the tailor-made force field and the hybrid method, a shortlist of crystal structures from a small energy window is selected for the final optimization.