Methods and applications of crystal structure prediction

11–13 July 2018
Cambridge, UK

Faraday Discussion

Wednesday 11 July

11.30	Registration, Tea and Coffee	
12.00	Lunch	
12.45	**Welcome and Introductions** Graeme Day, *Chair of Scientific Committee*	
12.55	**Outline of Discussion Format** Alexander Whiteside and Fiona Tscherny, *Royal Society of Chemistry Publishing Editors*	
13.00	**Introductory Lecture** (Session Chair: Graeme Day) Sarah L. Price *University College London*	
	Session 1: Structure searching methods (Session Chair: Christian Schön)	
14.00	**Accelerating CALYPSO structure prediction by data-driven learning of a potential energy surface** Yanming Ma *Jilin University*	**Paper 11894**
14.05	**Data-driven learning and prediction of inorganic crystal structures** Volker L. Deringer *University of Cambridge*	**Paper 19763**
14.10	**Evolutionary niching in the GAtor genetic algorithm for molecular crystal structure prediction** Noa Marom *Carnegie Mellon University*	**Paper 19768**
14.15	Discussion	
15.30	Afternoon tea	
	Session 1: Structure searching methods (Session Chair: Doris Braun)	
16.00	**TopoFF : MOF structure prediction using specifically optimized blue prints** Julian Keupp *Ruhr-Universität Bochum*	**Paper 19777**
16.05	**Zeolite structure determination using genetic algorithms and geometry optimisation** German Sastre *Instituto de Tecnologia Quimica UPV-CSIC*	**Paper 19660**
16.10	**The Flexible Unit Structure Engine (FUSE) for probe structure-based composition prediction** Christopher Collins *University of Liverpool*	**Paper 19676**
16.15	Discussion	
17.30	Lightning presentations (by invitation of the scientific committee)	
17.45	Poster Session and Wine Reception	
18.45	Close of Sessions	

Thursday 12 July

	Session 2: Crystal structure evaluation: calculating relative stabilities and other criteria (Session Chair: Aurora Cruz-Cabeza)	
09.00	**Identifying pragmatic quasi-harmonic electronic structure approaches for modeling molecular crystal thermal expansion** Gregory J. O. Beran *University of California, Riverside*	**Paper 11895**
09.05	**The importance of configurational disorder in crystal structure prediction: the case of loratadine** Grahame R. Woollam *Novartis*	**Paper 19774**
09.10	**Metashooting: a novel tool for free energy reconstruction from polymorphic phase transition mechanisms** Samuel A. Jobbins *Cardiff University*	**Paper 19673**
09.15	Discussion	
10.30	Morning Tea	
	Session 2: Crystal structure evaluation: calculating relative stabilities and other criteria (Session Chair: Caroline Mellot-Draznieks)	
11.00	**First-principles stability ranking of molecular crystal polymorphs with the DFT + MBD approach** Alexandre Tkatchenko *University of Luxembourg*	**Paper 11896**
11.05	**Crystal structure prediction of flexible pharmaceutical-like molecules: density functional tight-binding as an intermediate optimisation method and for free energy estimation** Jan Gerit Brandenburg *University College London*	**Paper 19408**
11.10	**Repulsion–dispersion parameters for the modelling of organic molecular crystals containing N, O, S and Cl** Claire S. Adjiman *Imperial College London*	**Paper 11893**
11.15	Discussion	
12.30	Lunch	
	Session 3: Applications of crystal structure prediction – organic molecular structures (Session Chair: Doris Braun)	
13.30	**Computational modelling of solvent effects in a prolific solvatomorphic porous organic cage** Andrew I. Cooper *University of Liverpool*	**Paper 11897**
13.35	**Towards the systematic crystallisation of molecular ionic cocrystals: insights from computed crystal form landscapes** Sharmarke Mohamed *Khalifa University of Science and Technology*	**Paper 19368**
13.40	**Predicting the structures and associated phase transition mechanisms in disordered crystals *via* a combination of experimental and theoretical methods** Michael T. Ruggiero *University of Cambridge*	**Paper 19612**
13.45	Discussion	

15.00	Afternoon Tea	
	Session 3: Applications of crystal structure prediction – organic molecular structures (Session Chair: Graeme Day)	
15.30	**How many ritonavir cases are there still out there?** Marcus A. Neumann *Avant-garde Materials Simulation*	**Paper 11898**
15.35	**Crystal structure prediction is changing from basic science to applied technology** Jonas Nyman *Eli-Lilly & Co and University of Wisconsin - Madison*	**Paper 19666**
15.40	**ROY revisited, again: the eighth solved structure** Qiang Zhu *University of Nevada Las Vegas*	**Paper 19696**
15.45	Discussion	
17.00	Poster session	
18.00	Close of Sessions	
18.30	Pre-Dinner Drinks	
19.00	Conference Dinner	

Friday 13 July

	Session 4: Applications of crystal structure prediction – inorganic and network structures (Session Chair: Aurora Cruz-Cabeza)	
09.00	**Reducing possible combinations of Wyckoff positions for zeolite structure prediction** Yi Li *Jilin University*	**Paper 11899**
09.05	**Materials discovery by chemical analogy: role of oxidation states in structure prediction** Daniel W. Davies *University of Bath*	**Paper 19691**
09.10	Discussion	
10.00	Morning Tea	
	Session 4: Applications of crystal structure prediction – inorganic and network structures (Session Chair: Caroline Mellot-Draznieks)	
10.30	**Adventures in boron chemistry – the prediction of novel ultra-flexible boron oxide frameworks** Frederik Claeyssens *University of Sheffield*	**Paper 19767**
10.35	**What is the best or most relevant global minimum for nanoclusters? Predicting, comparing and recycling cluster structures with WASP@N** Scott M. Woodley *University College London*	**Paper 19789**
10.40	Discussion	
11.30	**Concluding Remarks Lecture** (Session Chair: Christian Schön) Artem Oganov *Skolkovo Institute of Science and Technology*	
12.15	**Acknowledgements**	
12.25	**Close of meeting and Lunch**	

Presenting authors are indicated in the programme by an underline. The affiliation is for the presenting author. If the presenting author of your paper has changed since abstract selection please email events@rsc.org. Please note that this is a draft programme and timings may change.