BEST-CSP | COST Action CA22107

Bringing Experiment and Simulation Together in Crystal Structure Prediction

From molecules to materials:

2nd Workshop on

Benchmarking Solid State Properties

Book of Abstracts

10-11 September 2025 | Bologna, Italy

Organizing committee:

Fabrizia Grepioni (University of Bologna)
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Remie M. Sundermann (University of Parma)
Laura Contini (University of Bologna)

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Time	Wednesday 10/09	Title
8:00 am	REGISTRATION	
9:00 am	OPENING	
	Session Chairs:	**Michal Fulem, Joao Baptista**
9:15 am	KEYNOTE LECTURE: **Susan Reutzel Edens**	From digital design to the experimental realization of crystal polymorphs
10:00 am	Daria Szewczyk	Exploring Organic Crystalline Polymorphism through Heat Capacity Studies: Benzophenone, Picolinamide, Pyrazinamide, and Triethylenetetramine
10:15 am	Vera L.S. Freitas	When Intramolecular Hydrogen Bonds Undermine Crystal Cohesion: A Thermodynamic Perspective
10:30 am	Ricardo Castro	Discovery and Characterization of a Late-Appearing Polymorph of Famciclovir
10:45 am	Jonas Nyman	Blind test
11:00 am	COFFEE BREAK	
	Session Chairs:	**Anders Madsen, Inês Feliciano**
11:30 am	KEYNOTE LECTURE: **Mohamed Aouane**	Novel Materials: Opportunities with Neutron Scattering
12:15 pm	Ivor Loncaric	Modeling Molecular Crystals with Machine Learning Interatomic Potentials
12:30 pm	Vojtech Stejfa	From experiments to standard: reference data for sublimation properties
12:45 pm	Clara Gomes Mafalda Sarraguca	Women in STEM: Past, Present and Future
1:00 pm	LUNCH BREAK	
	Session Chairs:	**Sowmya Indrakumar, Luca Russo**
2:30 pm	KEYNOTE LECTURE: **Graeme Day**	Digital Navigation of Chemical-Crystal Space for Functional Materials Discovery
3:15 pm	Jacco van de Streek	Disorder, “correlated disorder”, energy and free energy
3:30 pm	Ctirad Cervinka	Coupled-clusters theory meets ab initio thermodynamic simulations for molecular liquids
3:45 pm	Demeter Tzeli	Computational Investigation of photophysical processes of chemosensors
4:00 pm	Pol Benitez	MLIPs for Crystal Prediction and Thermodynamic Phase Diagrams
4:15 pm	Lucia Gigli	Large-scale chemical and crystal packing space explora6on for HOF-based porous materials
4:30 pm	Zhuocen Yang	Relative Stability Evaluation of Polymorphic Systems via Pseudo-Supercritical Path Method using Different Force Fields
4:45 pm	COFFEE BREAK	
5:00 pm	POSTER SESSION	
6:30 pm	END of poster session	

Time	Thursday 11/09	Title
9:00 am	Management Committee Meeting	Management committee members only
10:00 am	Working Group Meetings	All participants
11:00 am	COFFEE BREAK	
11:30 am	Working Group Meetings	All participants
1:00 pm	LUNCH BREAK	
	Session Chairs:	**Helena Butkiewicz, Will Wood**
2:00 pm	KEYNOTE LECTURE: **Alberto de la Roza**	Design and benchmarking of methods for energy ranking in crystal structure prediction
2:45 pm	Natalia Correia	Exploring Crystal Polymorphism in Simvastatin: Insights from Dielectric Relaxation Spectroscopy
3:00 pm	Martin Dracinsky	NMR Crystallography of Molecular Solids with Strong Hydrogen Bonds
3:15 pm	Vassil Ivanov	Step Bunching and Meandering Dynamics: A pathway to surface morphology control
3:30 pm	Marta Dudek	NMR crystallography of organic solids at high magnetic fields
3:45 pm	Cheng-long Stephan	Stabilizing the Unstable: Using Additives to Control Metastable Polymorphs and Extend Their Lifetime
4:00 pm	COFFEE BREAK	
4:30 pm	Round Table Discussion	
5:45 pm	CLOSING REMARKS	
6:00 pm	Core Group Meeting	Core Group Members Only

Hierarchy of sigmoid growth models - towards justification of sigmoid treatment of nucleation data

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In the poster we provide a brief introduction to the general problem of fitting the nucleation data – the so called N-t curves, with an hierarchy of sigmoid growth models [1] (HSGM). The special focus of such a treatment is to be on the principal mechanisms of nucleation that could give raise to a positive feedback as demonstrated in the supelinear regime (before the inflection point) of N-t curves.

In the introductory part, we continue the mothodological development of the HSGM by identifying a novel quantitative criterium for "sigmoidness" based on the idea of catastrophe. Here we will use examples of population dynamics.

In the course of implementing the HSGM-approach we revisit several typical datasets reporting sigmoid data [2] and more. A novel tool used in the course of this revisit is the so called Multiple Fitting of a Single Dataset (MFSDS) as first proposed in [3]. Here we also make further refinements of the approach by including datasets generated by the Richards model and Cellular Automata.

In collaboration with: Daniela Tsekova and Feyzim Hodzhaoglu

References

[1] V. Kleshtanova, V. Ivanov, F. Hodzhaoglu, J. Prieto, and V. Tonchev, Heterogeneous Substrates Modify Non-Classical Nucleation Pathways: Reanalysis of Kinetic Data from the Electrodeposition of Mercury on Platinum Using Hierarchy of Sigmoid Growth Models, Crystals 13, 1690 (2023).

[2] C. N. Nanev and V. D. Tonchev, Sigmoid kinetics of protein crystal nucleation, Journal of Crystal Growth 427, 48 (2015).

[3] V. V. Ivanov, C. Tielemann, K. Avramova, S. Reinsch, and V. Tonchev, Modelling crystallization: When the normal growth velocity depends on the supersaturation, Journal of Physics and Chemistry of Solids 181, 111542 (2023).