

Navigating the Complexities of Crystallisation with CrystalGrower

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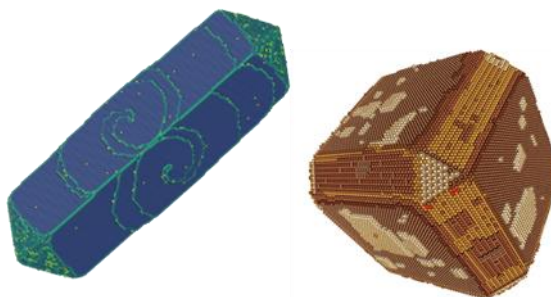
Abstract: Crystallisation, a fundamental yet intricate process, plays a crucial role in material science and industry. Despite its significance, understanding the multifaceted dynamics of crystallisation remains a challenge due to the myriad of parameters influencing the process. Small changes, such as altering the solvent, can drastically affect various factors including the free energy between building units, supersaturation levels, diffusion rates, and thermodynamic properties. Grasping these interconnections is essential for advancing in the field.

The CrystalGrower Workshop is designed to demystify the complexities of crystallisation through a hands-on, problem-solving approach. Utilizing the CrystalGrower software, participants will explore the journey of crystallisation from the foundational concepts of individual building units to the practical implications of growing crystals for industrial applications. This workshop aims to equip attendees with a deep understanding of crystallisation processes and the proficiency to employ CrystalGrower in addressing real-world challenges.^{1–3}

Participants will engage in a series of tutorials covering a broad spectrum of topics, including:

- Defining and manipulating building units.
- Analysing the impact of various interactions on crystallisation.
- Investigating solvent effects on crystal growth.
- Conducting morphology mapping to predict crystal shapes.
- Understanding the relationship between growth rates, thermodynamics, and crystal morphology.
- Applying seed engineering techniques to control crystallisation outcomes.

By the conclusion of this workshop, attendees will have acquired the knowledge and skills necessary to navigate the complexities of crystallisation, leveraging CrystalGrower to innovate and solve problems. This workshop is suited for researchers, academicians, and professionals seeking to enhance their expertise in crystallisation science and its applications.



References:

- A. R. Hill, P. Cubillas, J. T. Gebbie-Rayet, M. Trueman, N. de Bruyn, Z. A. Harthi, R. J. S. Pooley, M. P. Attfield, V. A. Blatov, D. M. Proserpio, J. D. Gale, D. Akporiaye, B. Arstad and M. W. Anderson, *Chem. Sci.*, 2021, 12, 1126–1146.
- M. W. Anderson, J. T. Gebbie-Rayet, A. R. Hill, N. Farida, M. P. Attfield, P. Cubillas, V. A. Blatov, D. M. Proserpio, D. Akporiaye, B. Arstad and J. D. Gale, *Nature*, 2017, 544, 456–459.
- P. R. Spackman, A. J. Walisinghe, M. W. Anderson and J. D. Gale, *Chem. Sci.*, 2023, 14, 7192–7207.

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