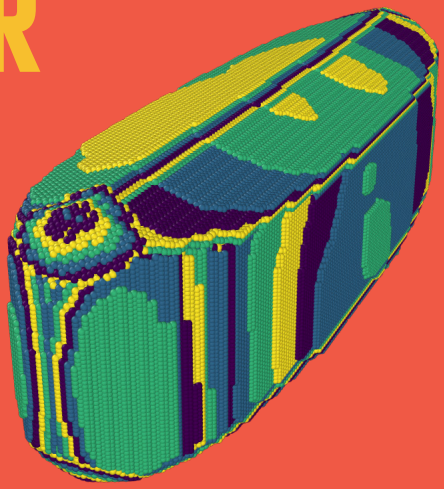
CRYSTAL GROWTH SIMULATION SOFTWARE

Generic Monte Carlo **crystal-growth software** for simulation of crystal habit and nanoscale surface topography

CrystoGen

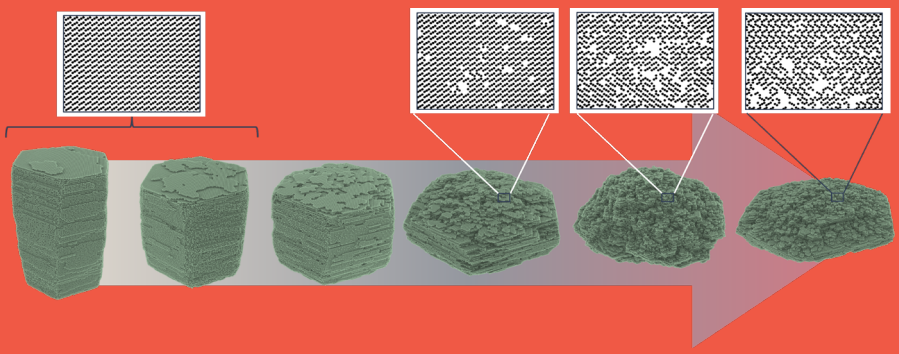
WANT TO UNDERSTAND HOW YOUR CRYSTALS GROW?



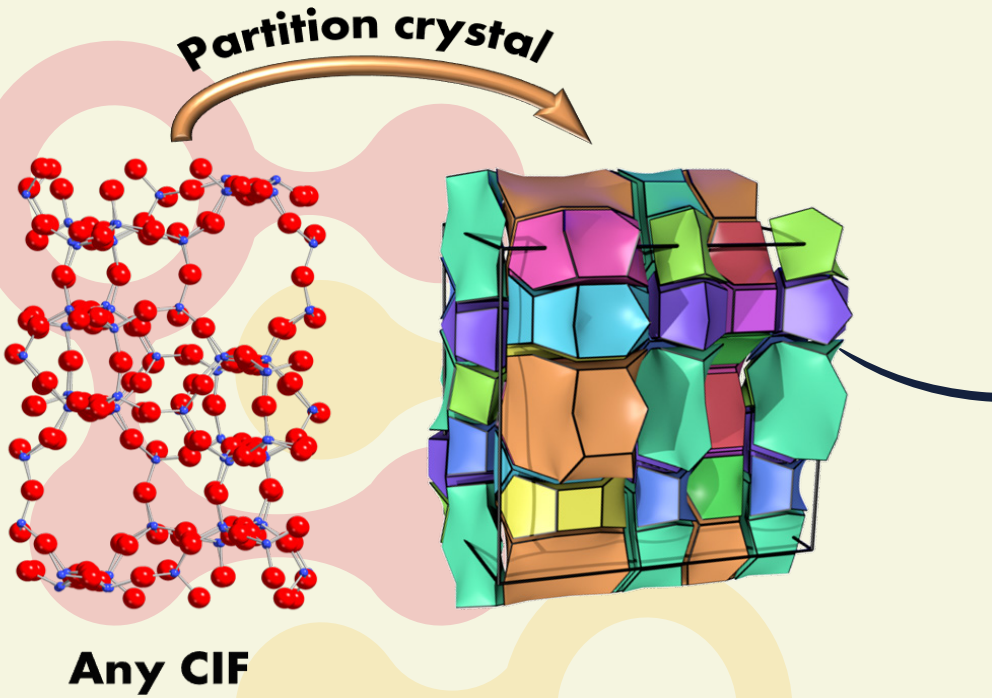
Understanding how crystals grow at the molecular scale is the key to **controlling crystal performance and functionality.** With the advent of scanning-probe microscopies the molecular details of surface topography are now accessible and, when **coupled** with the crystal habit, **provide a wealth of experimental information** that leads to this understanding**.** Our software is designed to help extract this information and maximise your knowledge of how your crystal system is behaving and, thereby, **tailor crystallisation conditions**.

PROBLEMS THAT CAN BE ADDRESSED:

- Crystal growth mechanism at the molecular scale
- Effect of supersaturation, temperature and solution speciation
- Effect of growth modifiers attaching to sites and surfaces
- Crystal habit and surface topography with nanoscale precision
- Screw dislocations, point defects and intergrowths
- Interfacial growth on a generic substrate surface

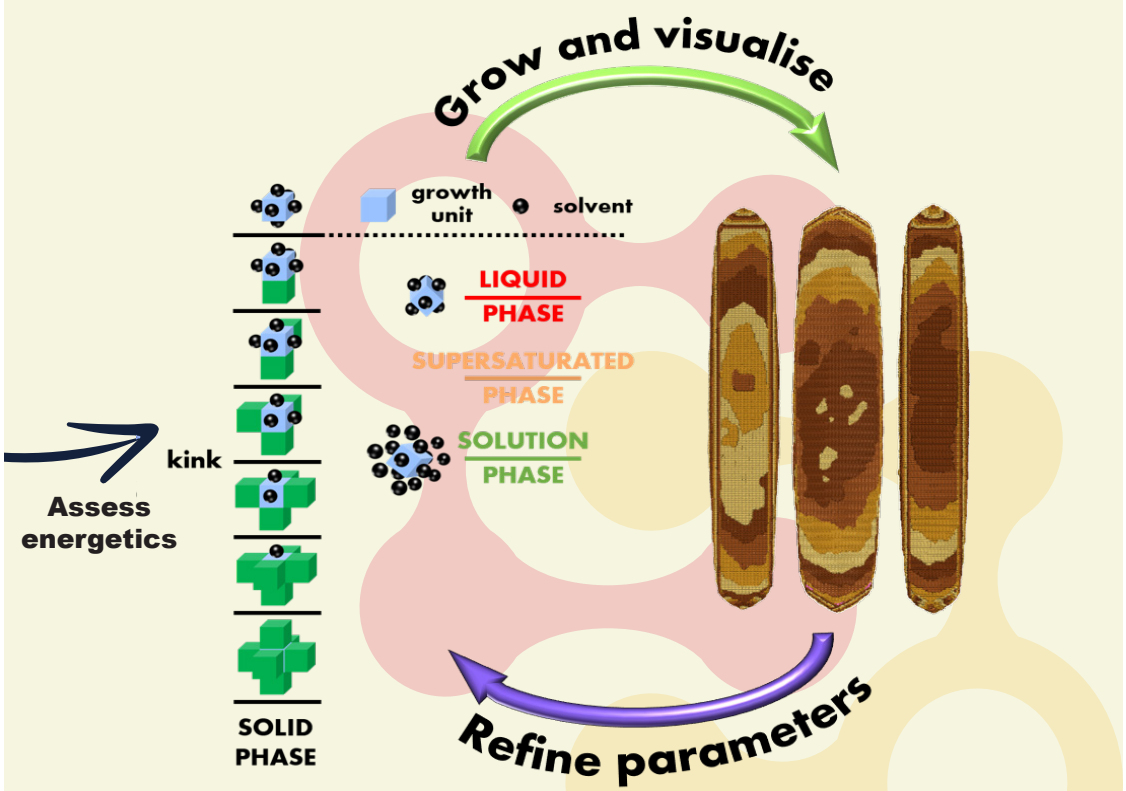


A SIMPLE MONTE CARLO METHODOLOGY

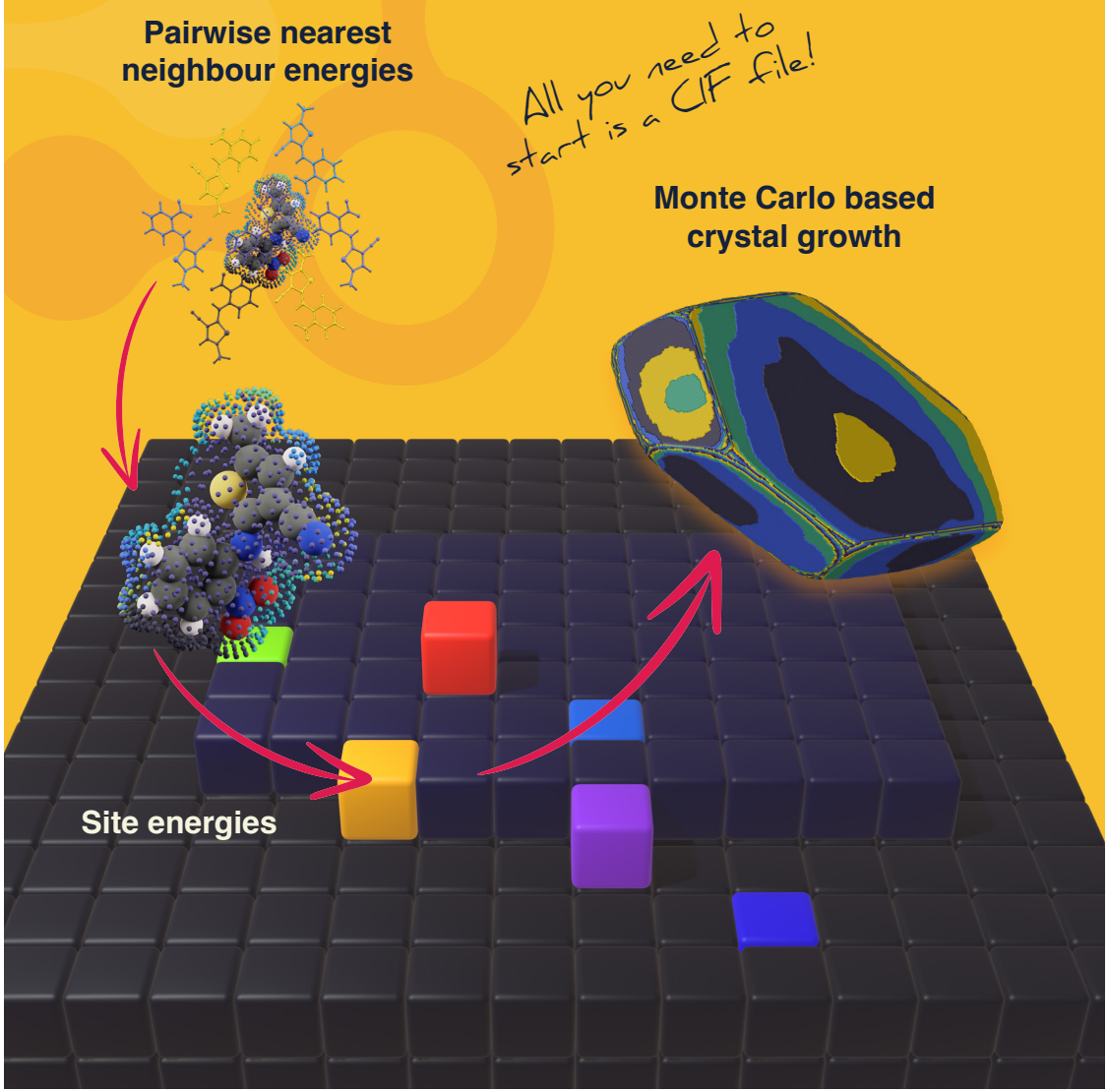


We have developed Monte Carlo and visualisation software, CrystoGen, that is able to **simultaneously simulate both crystal habit and nanoscale surface topography.** This is achieved for **any crystal structure under non-equilibrium conditions,** with the ability to add growth modifiers and to incorporate dislocations and defects.

Read the papers here



PAIRWISE INTERACTIONS DRIVING CRYSTAL GROWTH



WHO DOES IT BENEFIT?

Industries

Industrial professionals seeking to understand, control, and optimise crystallisation processes to reduce costs and improve product quality.

Academics

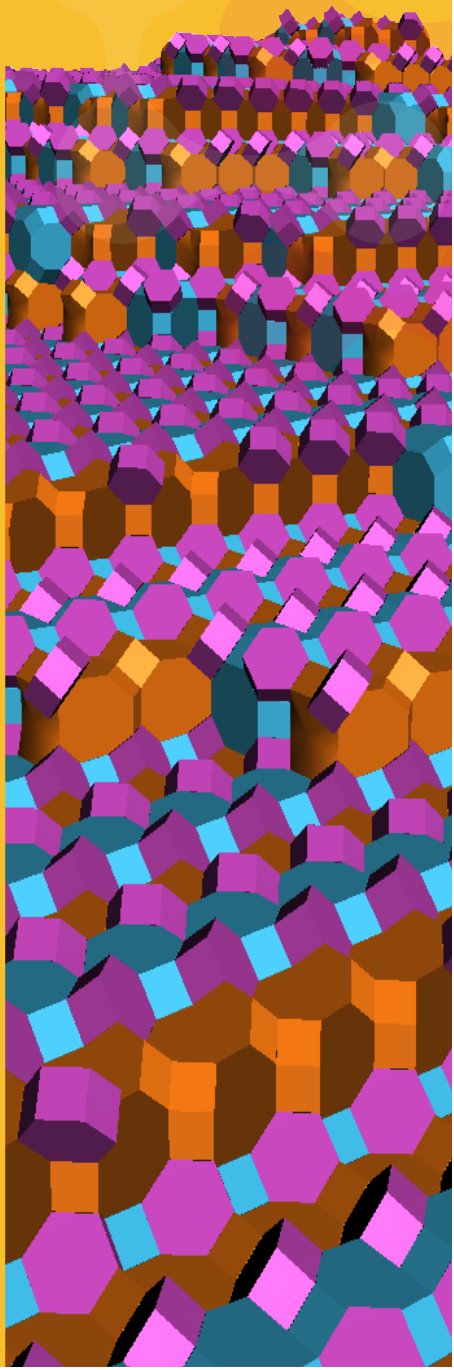
From PhD students and post-docs to leaders of their fields, anyone with an interest in the nanoscopic details of how ordered matter is formed.

Students

Undergraduates studying the chemistry and physics of crystallisation, along with any curious minds eager to dive deeper into the topic.

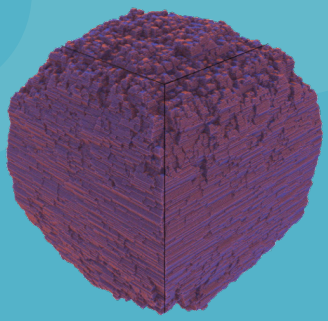
Educators

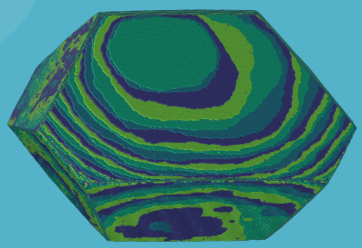
Schools and teachers looking to inspire young people with the beauty crystallisation. Our easy-to-use interface and fast simulations support teaching core concepts.

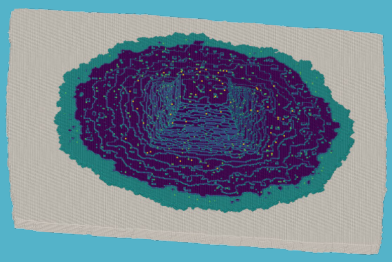


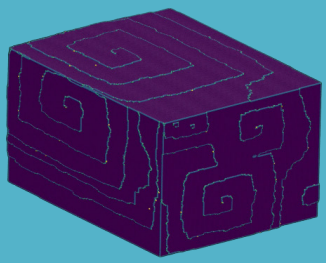
TYPES OF MATERIALS

Whether your interest is molecular crystals, co-crystals, ionic crystals, minerals, framework materials, metals or other crystal systems - **CrystoGen is the tool for you!**









EASE OF USE

Designing and understanding crystal morphologies shouldn't be a barrier. Our platform simplifies complex workflows, making advanced modelling intuitive, fast, and accessible to both experimentalists and theorists.

User-friendly interface

A streamlined environment designed for clarity and efficiency. Navigate complex simulations through a structured, visually guided workflow.

Insight-driven design

Go beyond visualisation. Translate interaction energies into meaningful crystal shapes and use them to guide experimental decisions with confidence.

Extensive video tutorials

Step-by-step guidance for every stage of the workflow. Learn quickly, troubleshoot easily, and get the most out of every feature.

Accesible

Whether you're at the bench or running simulations, the tool adapts to your expertise, thus lowering barriers without limiting capability.

Intuitive workflow

No steep learning curve! Just a clean, guided interface that lets you move from input to insight with minimal setup. Allowing you to focus on the science, not the software.

AWARD-WINNING PROGRESS IN CRYSTALLISATION

CrystoGen (formerly CrystalGrower) was recognised with the **Horizon Prize** for its innovative simulation capabilities. The award reflects both **advanced software development** and **international collaboration**.

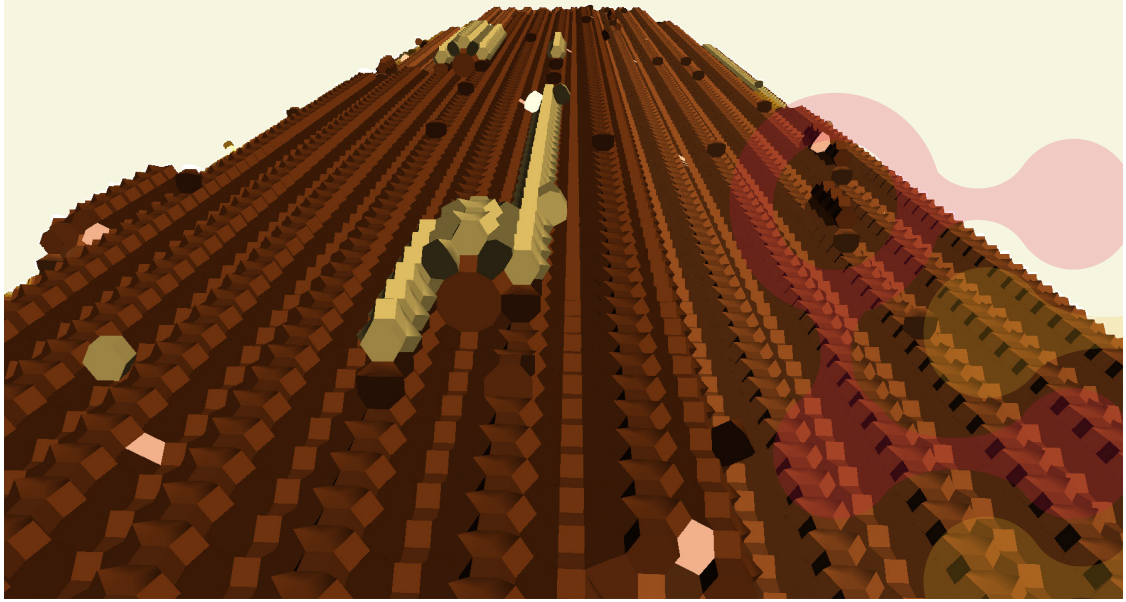
Watch the video to learn more

A SECURE PLATFORM

The **software runs entirely on your own computers** (laptop or super-computer) with **no web interface in order to provide a safe and secure environment** for your sensitive information.

FREE FOR ACADEMICS

Free for all academics and educators,
commercial users can contact **team@crystogen.org**



CONTACT US!

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