# Crystal Growth Simulation Software

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



# 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.





#### A simple Monte Carlo methodology

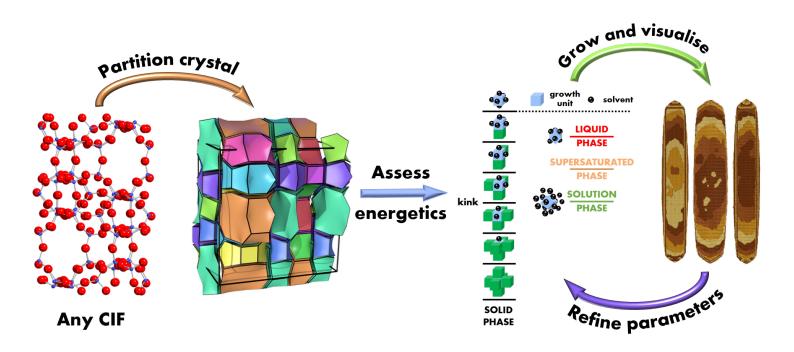
We have developed a Monte Carlo and visualisation software, CrystalGrower, that is *able to simultaneously simulate both crystal habit and nanoscale surface topography.* This is achieved for any crystal structure under non-equilibrium conditions, with the ability to add growth modifiers and to incorporate dislocations and defects. *The original concept is described in Nature,* 2017, 544, 456–459 and Chem. Sci., 2021, 12, 1126–1146



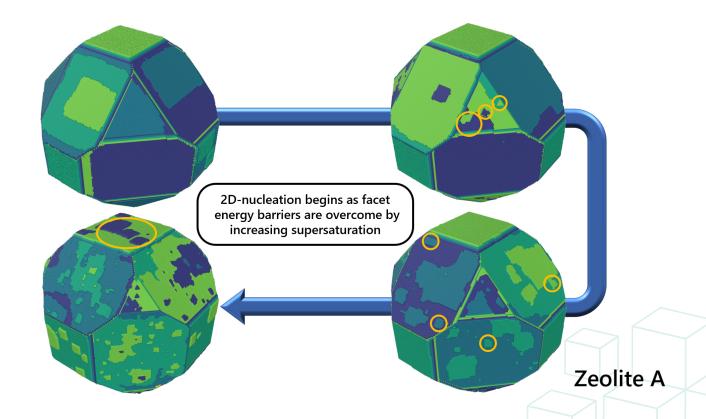
### Types of Materials:

Whether your interest is molecular crystals, co-crystals, ionic crystals, minerals, framework materials, metals or other crystal systems –

CrystalGrower is the tool for you!







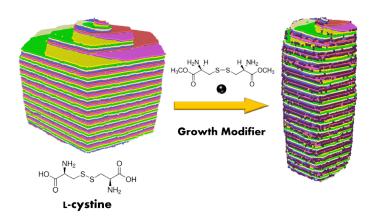
## Problems that can be addressed:

- ✓ Crystal growth **mechanism at the molecular scale**
- ✓ Crystal habit and surface topography with *nanoscale precision*
- ✓ Effect of supersaturation, temperature and **solution speciation**
- ✓ Effect of growth modifiers
- ✓ Screw dislocations, point defects and intergrowths

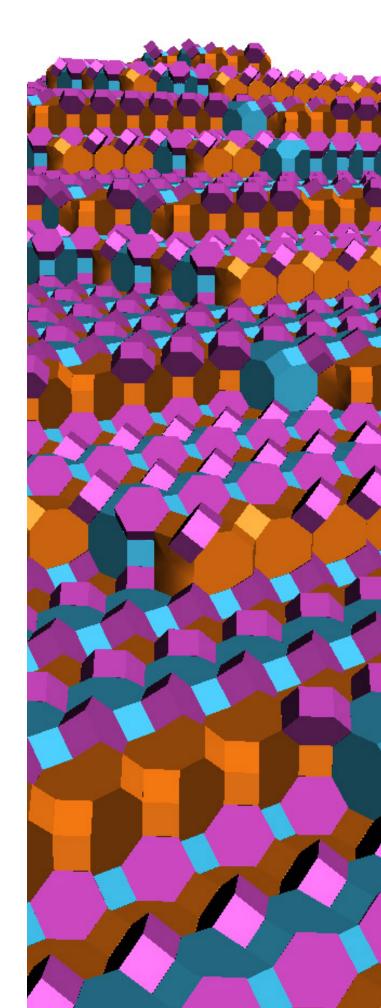


#### Ease of use:

We provide a user-friendly interface coupled with extensive video tutorials that are designed to make the tool accessible for all users, from bench-top experimentalists to theoreticians. Our goal is not only to deliver a better understanding of the crystal-growth mechanism but also to aid in the design of new and improved experimental methodologies that can be trialled in the laboratory.









#### 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.

#### Who does it benefit?

Industrialists who want to understand, control and modify crystallisation systems

Academics, PhD students and post-docs with an interest in the nanoscopic details of **how ordered matter is formed** 

**Undergraduates** who are studying the chemistry and physics of crystallisation

Educators interested to **teach young people** the importance and beauty of crystallisation

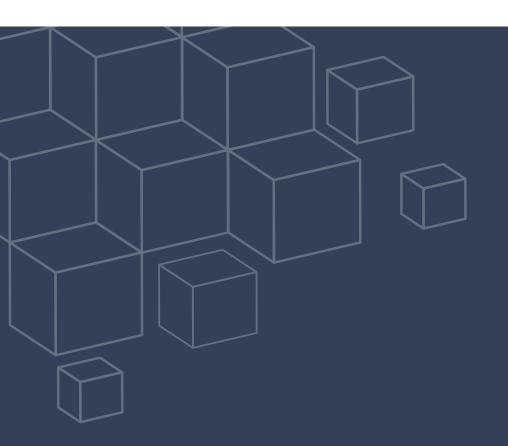
#### What's the Cost?

**Free** to academics and educators, commercial users please contact **team@crystalgrower.org** 





www.crystalgrower.org



#### Contact details:

- ( Website and software download: **crystalgrower.org**
- Youtube: <u>www.youtube.com/channel/CrystalGrower</u>
- Twitter: @crystalgrowerx
- e-mail: **team@crystalgrower.org**