

Avant-garde Materials Simulation

We are a self-funded

and Environment





a GRACE module

We have made Crystal Structures Predictable

We push frontiers to deliver In Silico Material Design

We bring genuine value to our customers by placing facts over fictions





















OUR TRACK RECORD

Used in >100/year industrial polymorph screens We have proven that the stable form is missing in 15-45% of the cases

Faraday Discussions doi.org/10.1039/C8FD00069G

CSP Factory, GRACE's core module achieved best results at the CCDC blind tests in 2024, 2015, 2010, 2007

doi.org/10.1107/S2052520624007492 doi.org/10.1107/S2052520624008679



CSP FACTORY

Is a fully automated software to generate crystal energy landscapes

Creates combined hydrate-anhydrate landscapes

Works for neat forms, co-crystals, solvates and salts of flexible molecules

Computes lattice free energies as a function of temperature and relative humidity with known error bars

Get your quote!

CSP Factory

will guide you

to new crystal forms

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