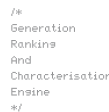


We are a self-funded family business

We push frontiers  
to deliver  
In Silico Material Design



GRACE CSP FACTORY

a GRACE module

We have made  
Crystal  
Structures  
Predictable

\* /

am polymorphic





$$G_{\alpha\beta}(\underline{r}, \underline{r}', t-t') = \begin{cases} \langle \hat{\psi}_{\alpha}^\dagger(t-t') / k \langle \hat{\psi}_{\alpha}^\dagger(\underline{r}) e^{-i\hat{H}(t-t')/k} \hat{\psi}_{\beta}^\dagger(\underline{r}') \rangle \rangle & t > t' \\ \langle \hat{\psi}_{\alpha}^\dagger(t-t') / k \langle \hat{\psi}_{\beta}^\dagger(\underline{r}') e^{-i\hat{H}(t-t')/k} \hat{\psi}_{\alpha}^\dagger(\underline{r}) \rangle \rangle & t < t' \end{cases}$$

$$G_{\alpha\beta}(\underline{r}, \underline{r}', \omega) = \int_{-\infty}^{\infty} d\tau G_{\alpha\beta}(\underline{r}, \underline{r}', \tau) e^{i\omega\tau}$$

$$\hat{\rho} = \sum_N \sum_{n_N=0}^{\infty} |n_N\rangle \langle n_N|$$

$$\hat{H}|n_N\rangle = E_{nN}|n_N\rangle, E_{nN} = E_n^* - E_0, |n_N\rangle = |n\rangle$$

$$\theta(\tau) = \lim_{\eta \rightarrow 0^+} \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \frac{e^{-i\omega'\tau}}{\omega + i\eta} \downarrow \Omega_n^* = E_n^* - E_0, \Omega_n^* = E_n^* - E_0$$

$$P_{\alpha\beta}(\underline{r}, \underline{r}', \omega) = \lim_{\eta \rightarrow 0^+} \sum_{n=0}^{\infty} \left\{ \langle \hat{\psi}_{\alpha}^\dagger(\underline{r}) | n_N \rangle \langle n_N | \hat{\psi}_{\beta}^\dagger(\underline{r}') \rangle \frac{\omega + \Omega_n^* + i\eta}{\omega - \Omega_n^* + i\eta} + \langle \hat{\psi}_{\beta}^\dagger(\underline{r}') | n_N \rangle \langle n_N | \hat{\psi}_{\alpha}^\dagger(\underline{r}) \rangle \frac{\omega + \Omega_n^* - i\eta}{\omega - \Omega_n^* - i\eta} \right\}$$

poles of Greens function  $\nearrow \text{Im (life time)}$

Chemical potential  $\mu$  excitation energy  $\epsilon$

## 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

Based on GRACE  
winner of the 2007, 2010 and 2015 blind tests on crystal structure prediction

Report on the sixth blind test  
doi.org/10.1107/S2052520616007447

## Get your map to new crystal forms



GRACE  
CSP FACTORY  
a GRACE module

## CSP FACTORY

Is a fully automated software to generate crystal energy landscapes

Creates combined hydrate-anhydrate landscapes

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

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

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poles of Greens function  $\nearrow \text{Im (life time)}$

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will guide you  
to new crystal forms

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