

/*

We are a self-funded family business

We are people-focused and care about Ethics and Environment

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GRACE

/*
Generation
Ranking
And
Characterisation
Engine
*/

GRACE
FORCE FIELD FACTORY

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

*/



/*
Avant-garde
Materials
Simulation
*/

I am polymorphic

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

Ab initio accuracy for large-scale molecular modelling



FORCE FIELD FACTORY

Is a fully automated software that derives tailor-made force fields from ab initio reference data

Supports atomic polarizabilities and electrostatic multipoles

Shifts transferability from force field parameters to the parameterization procedure

Exports force fields to LAMMPS, GROMACS, AMBER and Material Studio

Generates tailor-made force fields you can always trust

$$G_{\alpha\beta}(z, z', t-t') = \begin{cases} t > t': e^{-iE_0(t-t')/\hbar} \langle 0 | \hat{\psi}_{\alpha}(z) e^{-i\hat{H}(t-t')/\hbar} \hat{\psi}_{\beta}^{\dagger}(z') | 0 \rangle \\ t < t': e^{-iE_0(t-t')/\hbar} \langle 0 | \hat{\psi}_{\beta}^{\dagger}(z') e^{i\hat{H}(t-t')/\hbar} \hat{\psi}_{\alpha}(z) | 0 \rangle \end{cases} e^{i\omega\tau}$$

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

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

$$\downarrow \hat{H} |n_N\rangle = E_{nN} |n_N\rangle, E_{nN} z = E_n^{\pm}, |n_{N\pm}\rangle = |n\rangle$$

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

$$G_{\alpha\beta}(z, z', \omega) = \lim_{\eta \rightarrow 0^+} \sum_{n=0}^{\infty} \left\{ \langle 0 | \hat{\psi}_{\alpha}(z) | n_N \rangle \langle n_N | \hat{\psi}_{\beta}^{\dagger}(z') | 0 \rangle \frac{\langle 0 | \hat{\psi}_{\beta}^{\dagger}(z') | n \rangle \langle n | \hat{\psi}_{\alpha}(z) | 0 \rangle}{\omega - \Omega_n^+ + i\eta} \right. \\ \left. + \int_{-\infty}^{\infty} d\tau G_{\alpha\beta}(z, z', \tau) e^{i\omega\tau} \right.$$

poles of Green's function

$$\downarrow \Omega_n^+ = E_n^+ - E_0, \Omega_n^+ = E_n^+ - E_0$$

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

$$G_{\alpha\beta}(z, z', \omega) = \lim_{\eta \rightarrow 0^+} \sum_{n=0}^{\infty} \left\{ \langle 0 | \hat{\psi}_{\alpha}(z) | n_N \rangle \langle n_N | \hat{\psi}_{\beta}^{\dagger}(z') | 0 \rangle \frac{\langle 0 | \hat{\psi}_{\beta}^{\dagger}(z') | n \rangle \langle n | \hat{\psi}_{\alpha}(z) | 0 \rangle}{\omega - \Omega_n^+ + i\eta} \right. \\ \left. + \int_{-\infty}^{\infty} d\tau G_{\alpha\beta}(z, z', \tau) e^{i\omega\tau} \right.$$

poles of Green's function

$$\downarrow \Omega_n^+ = E_n^+ - E_0, \Omega_n^+ = E_n^+ - E_0$$