/*
Avant-garde
Materials
Simulation
*/

/*
We are a self-funded
family business

We are people-focused
and care about Ethics
and Environment
*/

GRACE

/*
Generation
Ranking
And
Characterisation
Ensine
*/

GRACE
FORCE FIELD FACTORY

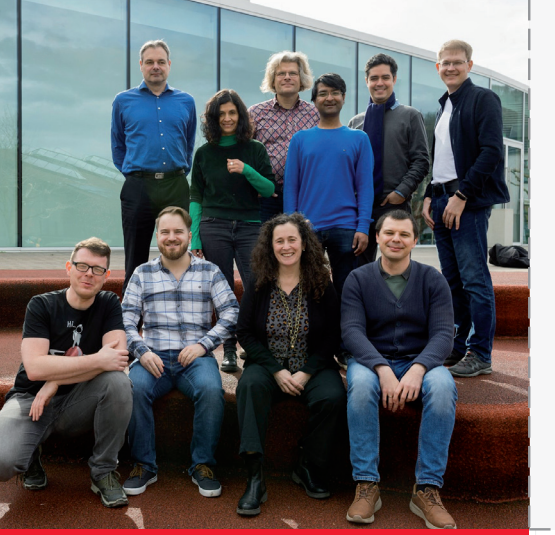
a GRACE module

/*
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
*/

I am polymorphic



OUR TRACK RECORD

Transferable Tailor-Made Force Fields for efficient CSP

https://pubs.acs.org/doi/10.1021/acs.jctc.2c00451

Tailor-Made Force Fields: a key component to generate crystal energy landscapes you can TRHu(ST)

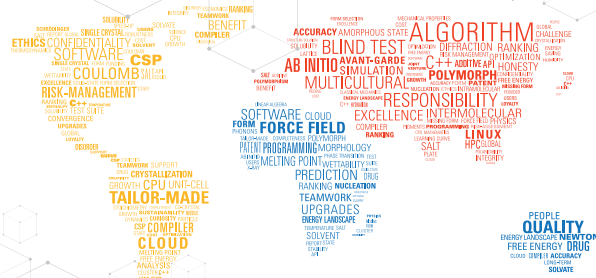
Predicting crystal form stability under real-world conditions

https://www.nature.com/articles/s41586-023-06587-3

Since 2008, we have been generating proprietary Tailor-Made Force Fields

https://doi.org/10.1021/jp710575h

Ab initio accuracy for large-scale molecular modelling



GRACE
FORCE FIELD FACTORY

a GRACE module

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 use with TRHu(ST)

Get your quote!
Force Field Factory
now brings our tailor-made force fields
to your favorite molecular
simulation engine

E quotes@avmatsim.eu
T + 49 (0)761 479984-0
www.avmatsim.eu

Avant-garde Materials Simulation Deutschland GmbH
Local Court Freiburg HRB 701900 | Tax ID DE 259 132 789
Alte Straße 2 | 79249 Merzhausen | Germany
CEOs Dr. Marcus Neumann, Elsa Gheziel M. A.