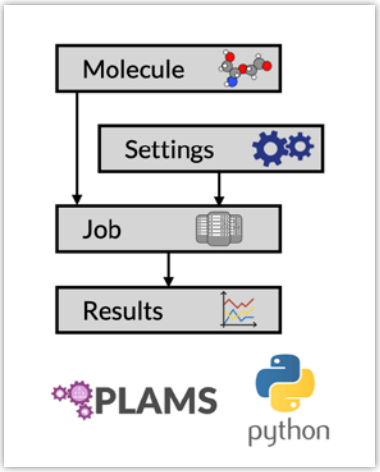
Scripting
with the Amsterdam Modeling Suite

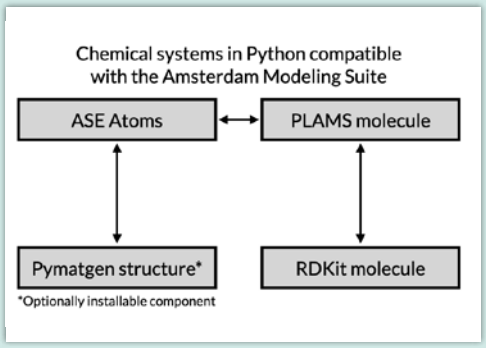
Python Library for Automating Molecular Simulations (PLAMS)

Enhance your molecular simulations with PLAMS, our dedicated Python interface for the Amsterdam Modeling Suite. Simplify the setup, execution, and analysis of complex calculations with automatic workflows, ensuring reproducibility and eliminating human error. Scale up your research with high-throughput screening of molecules and materials.



What can you do with PLAMS?

- Define the atomic structure (easily specify molecules, crystals, surfaces, and more)
- Configure simulation parameters with ease
- Execute single jobs or multiple jobs in parallel seamlessly
- Perform comprehensive analysis and plotting of your simulation data
- Design intricate multi-step calculation workflows
- Utilize Jupyter notebooks for interactive coding and documentation

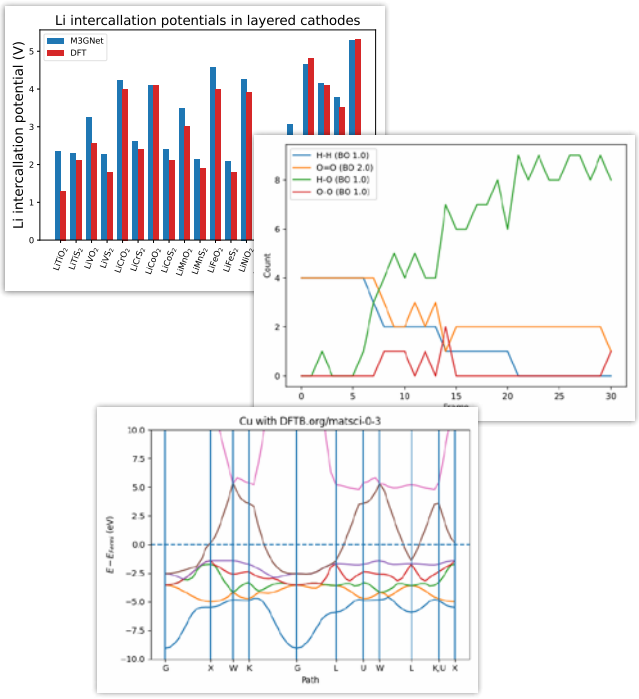


Key features of PLAMS

- √ ASE interface, molecule class, packmol interface (efficiently handle packing of molecules into defined structures)
- √ Benefit from hassle-free management of files and folders
- √ Run jobs in parallel without special parallel scripting
- √ Save GUI settings directly into PLAMS
- √ Leverage the Python Input System for AMS (PISA) with autocompletion and runtime validation

Examples

- Analyze molecular properties, bonds, and rings along a simulation trajectory
- Automate the substitution of ligands in molecules
- Calculate diffusion, ionic conductivity, IR spectra, redox potentials, and more
- Generate and evaluate molecular conformers
- Visualize electronic band structures or phonons
- Optimize ReaxFF parameters and Machine Learning Potentials
- Perform active learning for enhanced simulations



SCM
Software for Chemistry & Materials

Explore Scripting with AMS

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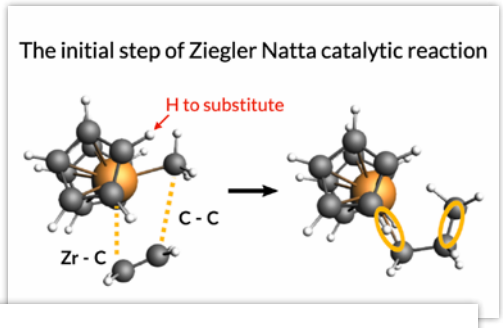
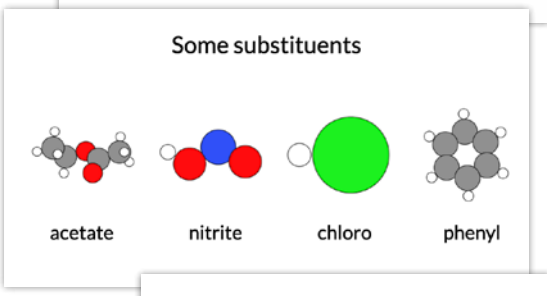
Ziegler Natta Catalyst

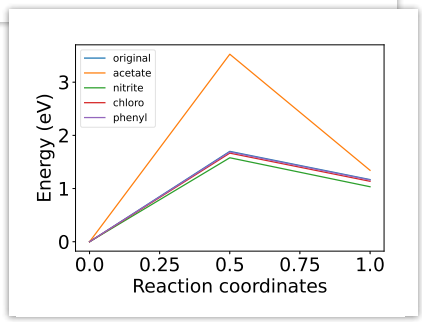
Discovered by Karl Ziegler and first applied to polymerization by Giulio Natta, this class of catalysts soon became an industry standard for the production of various polyolefins. Consequently, Ziegler and Natta's work was awarded a Nobel Prize in 1963. Nowadays, the industrial Ziegler-Natta polymerization of polyolefins is among the most important industrial processes. We show here that using PLAMS you can easily screen catalysts to optimize their chemical reaction.





Methods and results

The workflow starts from a transition state (TS). This TS can be obtained by first scanning proper coordinates along the reactant and product geometries (also possible with NEB and PES exploration). Then selecting the saddle point to optimize the TS geometry. Second, the user must define the atom that will be substituted. Third, an ensemble of substituents is defined. Finally, the PLAMS script proceeds by substituting the H atom of the TS geometry with each ligand and computing the energies of the reactant, product and TS. This can be scaled-up to screen thousands, or even millions of potential ligands in order to tune the catalytic reaction.



"What I really like about the Amsterdam Modeling Suite is that the programs were clearly written by chemists for dealing with real chemical problems. A great suite of programs!"

– Roald Hoffmann, Nobel Laureate

About SCM

Scientists at SCM are passionate about making computational chemistry work for you. Our mission is to develop powerful, easy-to-use software for your research and development needs. We love to discuss your research and learn how we can serve you better in the future.

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