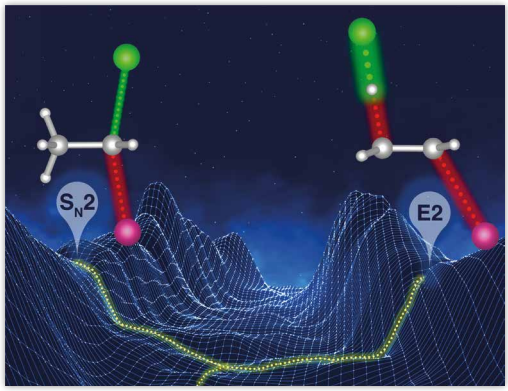
Bonding & Reactivity
with the Amsterdam Modeling Suite

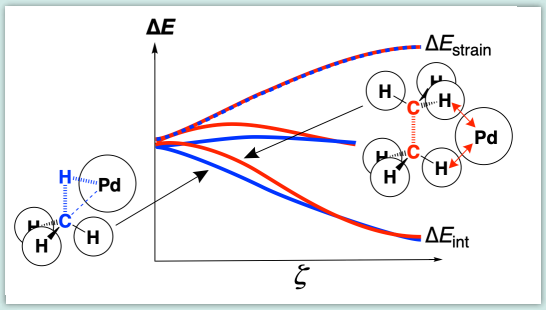
Understand mechanisms and processes, at the atomic scale

Our advanced density functional theory codes, ADF and BAND, are equipped with powerful analysis tools that provide unparalleled insight into chemical bonding, reactivity, and critical properties such as charges, electron densities, and potentials. The intuitive GUI seamlessly integrates these analysis features, allowing you to visualize complex results effortlessly and with clarity.

What can you compute with AMS?

- Automated activation strain analysis of reactions
- Energy decomposition analysis (EDA) for detailed bond insights
- Orbital interaction analysis based on fragment orbitals
- Voronoi deformation density (VDD) analysis of bonds
- Atomic charges: VDD, Hirshfeld, MDC, Mulliken, CM5
- Transfer integrals to assess charge mobility and bonding
- Advanced analyses: NBO, QTAIM, ETS-NOCV, IQA, NCI, Fukui
- Aromaticity indices



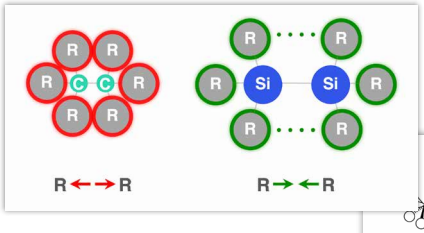


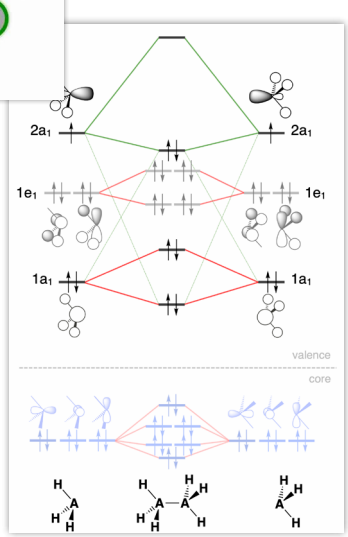
Key methods for Bonding & Reactivity

- √ Easy visualization and analysis in integrated GUI
- √ Automated activation strain analysis (PyFrag)
- √ Bond energy decomposition analysis (EDA)
- √ Quantitative molecular orbital diagrams
- √ Efficient exploitation of symmetry in calculations
- √ Advanced VDD charge density analysis

Tools and analysis for Bonding & Reactivity

- Understand bonding and orbital hybridization with AMSlevels
- Visualize molecular orbitals, spin density, and more with AMSview
- Explore dynamic trajectories with AMSmovie
- Unlock advanced computational insights with PyFrag and PyOrb (coming soon)





SCM
Software for Chemistry & Materials

Explore Bonding & Reactivity with AMS

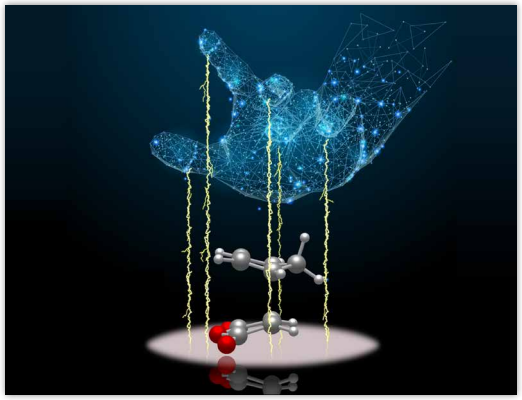
Bonding & Reactivity

with the Amsterdam Modeling Suite

SCM
Software for Chemistry & Materials

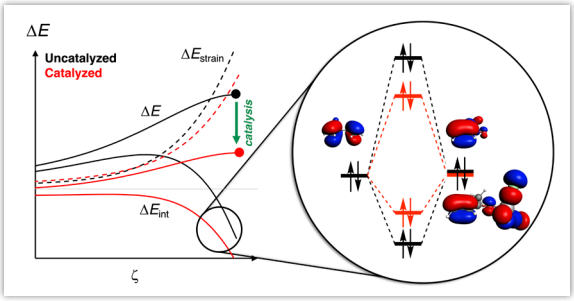
Rational design & teaching

Achieve cost-efficient development of novel high-performance materials and sustainable processes in fine and bulk chemicals or pharmaceuticals with the predictive power and deep understanding provided by ADF and BAND. Whether you're advancing cutting-edge research or exploring the fundamentals of chemistry and material science, these tools empower both innovation and education.



Synthesis & homogenous catalysis

Homogeneous catalysis offers a prime example of advanced molecular design, from selective and active transition-metal complexes in cross-coupling reactions to organocatalysts in electrocyclic processes, or even artificial enzymes. With activation-strain analysis and quantitative MO concepts, you can design the optimal system from the start, then fine-tune it computationally before heading to the lab, saving time and resources.



"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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