

CMM research

The mission of the CMM is to use molecular modeling as the central instrument for the characterization, understanding and design of materials and chemical processes. The CMM consists of strongly interacting research cells (depicted in the figure above) that are embedded in a network of partners at the Ghent University, in Flanders, and at an international level.

Interdisciplinary research is stimulated by the synergy between the different research branches, the diverse backgrounds of its members (chemistry, physics, engineering and biochemistry), and the large number of collaborations with experimental research groups. As the CMM is composed of theoretical and computational divisions, new model developments can immediately be employed in the more application driven areas and this allows to go beyond state of the art. It is precisely this multidisciplinary character of the CMM, which is the key towards excellence. In some areas the CMM has acquired a prominent position illustrated by various papers published in top journals on an annual basis.



HiPart

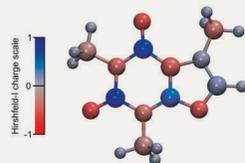
HiPart is a program to analyze the electronic structure of molecules with fuzzy-atom density partitioning methods.

Features

- Becke, Hirshfeld, Hirshfeld-I and ISA partitioning
- Atoms-in-molecules (AIM) properties:
 - Atomic charges and dipoles
 - Quality of charges and dipoles with respect to the ESP
- Full atomic multipole expansions
- Net and overlap populations
- Bond orders
- Spin charges

Example script (bash)

```
# Create database of atomic densities (densities.txt)
hi-atomdb.py g09 'B3LYP/6-311+G**' 1,6-8
# Compute partial charges with the Hirshfeld-I scheme
hi-charges.py caffeine.fchk hirshi densities.txt
```



Strengths and prospects

Any partitioning scheme can be combined with any atoms-in-molecules (AIM) property. Furthermore HiPart is our framework to develop new partitioning schemes. We are currently preparing a new release with two new partitioning schemes and more AIM properties.

Contact information

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BELGIUM

CMM Software

June 2012

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The CMM software is made by and for researchers in the field of molecular modeling. The development of this software is driven by our need for advanced computational tools in the CMM research activities. Our general philosophy is to provide added value in the preparation and post-processing of molecular simulations. All packages have a modular and flexible design, making them applicable in diverse types of research projects, such as level-of-theory studies, the analysis of reaction mechanisms, decomposing vibrational spectra, and so on.

We choose to generously share these computational tools with the scientific community as free software (GPLv3), provided that one makes proper citations. This flyer gives a condensed overview of our main software packages.

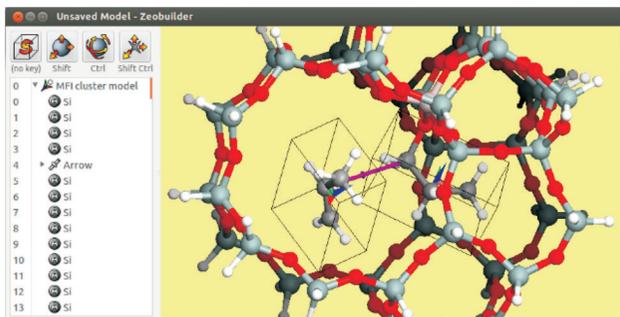
<http://molmod.ugent.be>



Zeobuilder is a user-friendly GUI toolkit for the construction of any type of advanced molecular structure (biological, inorganic, nanoporous materials, ...).

Features

- Composition & alignment of molecular fragments
- Hierarchical reference frames
- Advanced builder tools (nanotube generator, ...)
- Topological and structural analysis
- Extensible through plug-ins



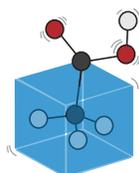
Strengths

- Any number of molecules can be imported and used to compose a molecular system.
- The graphical interface gives fine-grained control over geometrical transformations of building blocks.

Reference: Verstraelen, T.; Van Speybroeck, V.; Waroquier, M. "ZEOBUILDER: A GUI Toolkit for the Construction of Complex Molecular Structures on the Nanoscale with Building Blocks" *J. Chem. Inf. Model.* **2008**, 48, 1530-1541.

MolMod library

MolMod is the underlying Python library for Zeobuilder, TAMkin, HiPart, MD-Tracks and other projects at the CMM. It contains several auxiliary modules for the development of molecular modeling programs.

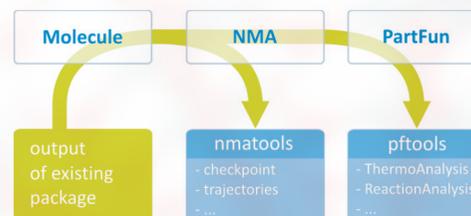


TAMkin

TAMkin is a post-processing toolkit for normal mode analysis, thermochemistry, and reaction kinetics.

Features

- Supports output from CHARMM, CP2K, CPMD, GAMESS, GAUSSIAN, QCHEM, and VASP
- Methods for Normal Mode Analysis (NMA): Partial Hessian Vibrational Analysis (PHVA), Mobile Block Hessian (MBH), Vibrational Subsystem Analysis (VSA),...
- Flexible definition of partition functions
- Derivation of thermodynamic and kinetic parameters



Example script (python)

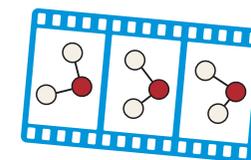
```

from tamkin import *
# Load Gaussian03 output
mol_react = load_molecule_g03fchk("butadiene.fchk")
mol_prod = load_molecule_g03fchk("cyclobutene.fchk")
# Perform normal mode analysis
nma_react = NMA(mol_react, ConstrainExt())
nma_prod = NMA(mol_prod, ConstrainExt())
# Construct partition functions
pf_react = PartFun(nma_react, [ExtTrans(), ExtRot()])
pf_prod = PartFun(nma_prod, [ExtTrans(), ExtRot()])
# Study reaction thermodynamics
tm = ThermodynamicModel([pf_react], [pf_prod])
print tm.free_energy_change(500) # at 500 Kelvin
  
```

Strengths

- Any combination of simulation output, NMA method and partition function is allowed.
- The scripting interface imposes a well-defined computational protocol (e.g. for a level-of-theory study).

Reference: Ghysels, A.; Verstraelen, T.; Hemelsoet, K.; Waroquier, M.; Van Speybroeck, V. "TAMkin: A Versatile Package for Vibrational Analysis and Chemical Kinetics" *J. Chem. Inf. Model.* **2010**, 50, 1736-1750.

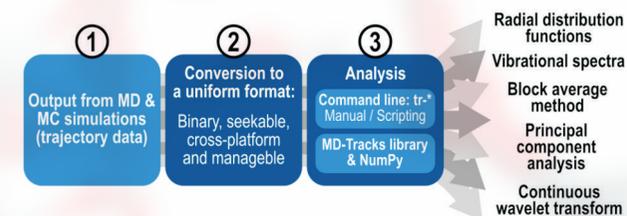


MD-Tracks

MD-Tracks is a trajectory analysis toolkit for molecular dynamics and Monte Carlo simulations.

Features

- Conversion of trajectory data into a binary format (CP2K, CPMD, DLPOLY, GROMACS, LAMMPS)
- Collection of analysis scripts that operate on the binary data
- Vibrational analysis
- Radial distribution functions
- Diffusion coefficients
- Principal component analysis



Example script (bash)

```

# Convert trajectory data from CP2K
tr-from-xyz md-vel-1.xyz vel -u au
tr-from-cp2k-ener md-1.ener
# Perform Spectrum analysis (FFT)
tr-spectrum tracks/atom.vel.* tracks/time sliced/s
# Plot result
tr-plot :line tracks/s.wavenumbers tracks/s.amplitude \
--xlim=0,4000*invcm --xunit=invcm
  
```

Strengths

- The binary trajectory format is cross-platform.
- Complex analysis scripts may be constructed by using the output of one script as input for a subsequent script.

Reference: Verstraelen, T.; Van Houteghem, M.; Van Speybroeck, V.; Waroquier, M. "MD-TRACKS: A Productive Solution for the Advanced Analysis of Molecular Dynamics and Monte Carlo simulations" *J. Chem. Inf. Model.* **2008**, 48, 2414-2424.