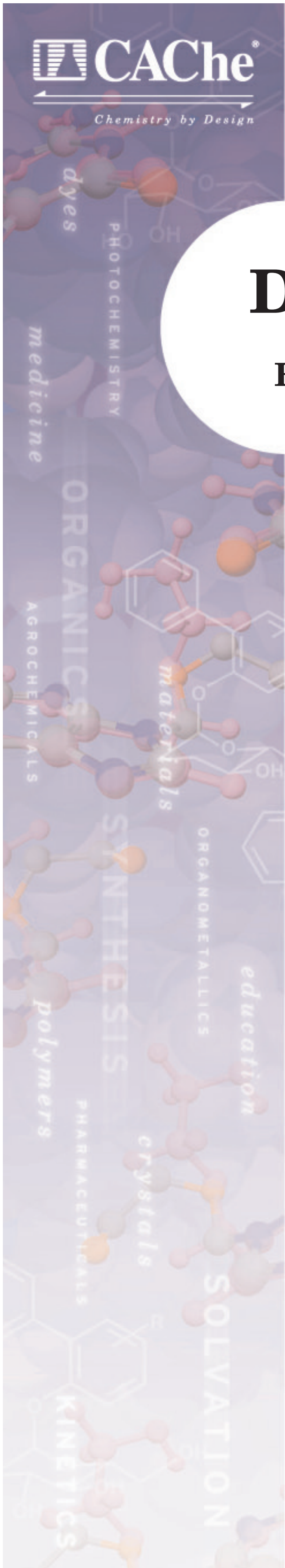


High - Performance Quantum Mechanics

DGauss Compute Engine

High-Performance Quantum Mechanics ... on Your Windows Desktop

DGauss is a high-accuracy compute engine that uses density functional theory (DFT) to predict molecular structures, properties and energetics. The ease-of-use available within the *ab initio* CAChe and CAChe WorkSystem Pro packages coupled with DGauss' high-performance offers

- **High Speed**. DGauss can be more than 10 times faster than competing programs.
- **High Accuracy**. DGauss predicts energies, structures and properties significantly more reliably than semiempirical methods, approaching MP2 in accuracy.
- **Broad Applicability**. DGauss works for organic, inorganic and organometallic compounds.

DGauss Benefits

- **Transition Metal Chemistry**

  DGauss accurately models metal compounds, such as metallo-enzymes and organometallics. Using DGauss to predict structures, energies, and electronic properties of metal containing compounds, you can elucidate catalytic mechanisms and accelerate the design of novel catalysts.

- **Large Molecule Analysis**

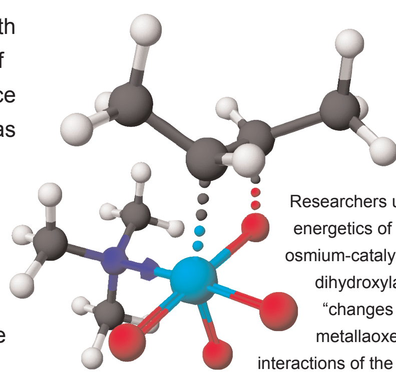
  DGauss can be applied to very large molecular systems–even calculations with over one hundred atoms or thousands of basis functions are possible. Performance scales well on multiprocessor systems, as shown in the table on the reverse. By studying larger systems, you can create more realistic models and tackle more complex processes, all important considerations when attempting to produce results that must be comparable to experimental results.

- **Transition States and Kinetics**

  DGauss calculations of activation energies and analytic second derivatives permit analysis of reaction mechanisms by providing accurate location and characterization of transition states. Performance can be up to 50 times faster than other methods. Using this knowledge, you can understand reaction rates and engineer reactions to obtain more desirable results.

- **IR and NMR Spectra**

  IR spectra predictions are typically within 5% of experiment. In addition, DGauss computes NMR absolute shielding constants using IGLO and LORG methods.



Researchers used DGauss to study the energetics of high enantioselective osmium-catalyzed asymmetric dihydroxylation. They discovered that "changes in the puckering of the metallaoxetane, together with interactions of the substrate with the 'binding pocket' of the ligand, seem to be responsible for the selectivities observed for olefin substitution patterns". (Norrby, Becker, and Sharpless, JACS 1996, 118, 35-42)

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DGauss Features

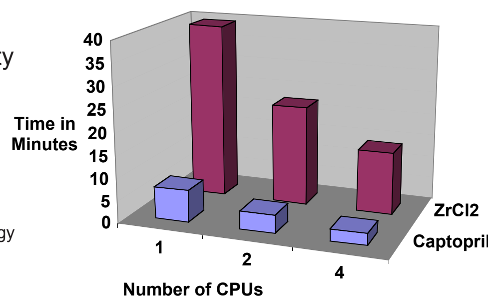
Density Functional Calculations

- Spin-restricted for closed-shell
- Spin-unrestricted for open-shell
- Harris approximation
- LDA and GGA exchange-correlation functionals
- Relativistic pseudopotentials, all elements H to La and Hf to Rn
- Analytic second derivatives (except for pseudo-potential systems)
- All atoms except the Lanthanides and Actinides
- Dummy atoms can be used to improve the ease and versatility of geometry optimizations

Property Predictions

- IR frequencies and intensities
- Raman frequencies
- NMR shielding constants
- Population analysis
- Multipole moments
- Photoelectron spectra
- Density of states (DOS)
- Electrostatic potential fit charges
- Geometry optimizations to both minima and transition states

The table below shows the time required to complete a series of GGA single-point energy calculations on three molecules of different complexity. DGauss scales efficiently on multiprocessor systems.



Elapsed Time (Minutes)								
	System:	Intel Pentium III 733 MHz		Intel Xeon 1.7 GHz		SGI R12000 300 MHz		
Molecule	# of processors:	1	2	1	2	1	2	4
Captopril		9.8	5.8	4.8	2.9	7.2	4.1	2.7
$ZrCl_2$		54.8	34.2	25.3	15.3	39.4	22.4	13.9
LC Dimer		(not available)		(not available)		410.7	264.4	200.1

Details for Performance Calculations

Molecule	Formula	Atom Count	Basis Functions	Quadrature Points	SCF Iteration
Captopril	$C_9H_{15}NO_3S$	29	244	34K	13
First orally active inhibitor of angiotensin-converting enzyme					
$ZrCl_2$	$ZrCl_2C_{21}H_{18}$	42	428	51K	15
Cyclopentadienyl zirconium dichloride, a catalyst for stereo-specific polymerization reactions					
LC Dimer	$C_{48}H_{46}O_{12}Cl_2$	108	1030	127K	19
A liquid crystal dimer					

System & Software Requiremets

Windows
One or more Intel Pentium family processors

Windows NT / 2000

SGI
IRIX 6.5

IBM
RS/6000 with AIX 4.3
(Also runs on an SP system, but only on individual nodes)

Recommended Resources (all systems)
At least 64 MBytes of physical memory
256 MBytes of swap space (where applicable)

Software
DGauss is available within *ab initio* CAChe and CAChe Worksystem Pro

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