List of quantum chemistry and solid-state physics software

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Quantum chemistry computer programs are used in computational chemistry to implement the methods of quantum chemistry. Most include the Hartree–Fock (HF) and some post-Hartree–Fock methods. They may also include density functional theory (DFT), molecular mechanics or semi-empirical quantum chemistry methods. The programs include both open source and commercial software. Most of them are large, often containing several separate programs, and have been developed over many years.

The following table illustrates some of their main capabilities.

Package	License†	Language	Basis	Periodic‡	Mol. mech.	Semi-emp.	HF	Post-HF	MRCI	DFT	GPU
ABINIT	Free, GPL	Fortran	PW	3d	Yes	No	No	No	No	Yes	Yes
ACES	Free, GPL	Fortran, C++	GTO	No	No	No	Yes	Yes	No	Yes	Yes
ACE-Molecule	Free, GPL	C++	Grid, Lagrange function(Sinc)	Any[15]	No	Yes	No	Yes	No	Yes	Yes, CUDA
AMPAC	Academic	Unknown	Unknown	Unknown	No	Yes	No	No	No	No	No
ADF	Commercial	Fortran	STO	Any	Yes	Yes[4]	Yes	No	No	Yes	Yes
Atomistix ToolKit (ATK)	Commercial	C++, Python	NAO, EHT, PW	Any[9]	Yes	Yes	No	No	No	Yes	No
BigDFT	Free, GPL	Fortran	Wavelet	Any	Yes	No	Yes	No	No	Yes	Yes
BrianQC	Commercial	C++, CUDA	GTO	No	Yes	No	Yes	No	No	Yes	Yes
CADPAC	Academic	Fortran	GTO	No	No	No	Yes	Yes	No	Yes	No
CASINO (QMC)	Academic	Fortran 95	GTO, PW, Spline, Grid, STO	Any	No	No	Yes	Yes	No	No	No
CASTEP	Academic, commercial	Fortran 95, Fortran 2003	PW	3d	Yes	No	Yes[5]	No	No	Yes	No
CFOUR	Academic	Fortran, C++	GTO	No	No	No	Yes	Yes	No	No	No
COLUMBUS	Academic	Fortran	GTO	No	No	No	Yes	Yes	Yes	No	No
CONQUEST	Academic	Fortran 90	NAO, Spline	3d	Yes	No	Yes[5]	No	No	Yes	No
CP2K	Free, GPL	Fortran 95	Hybrid GTO, PW	Any	Yes	Yes	Yes	Yes	No	Yes	Yes, CUDA and OpenCL
CPMD	Academic	Fortran	PW	3d	Yes	No	Yes	No	No	Yes	No
CRYSTAL	Academic (UK), commercial (IT)	Fortran	GTO	Any	Yes	No	Yes	Yes[10]	No	Yes	No
DACAPO	Free, GPL?[1]	Fortran	PW	3d	Yes	No	No	No	No	Yes	No
Dalton	Free, LGPL	Fortran	GTO	No	No	No	Yes	Yes	Yes	Yes	No
deMon2k	Academic, commercial	Fortran	GTO	No	Yes	No	No	No	No	Yes	No
DFTB+	Free, LGPL	Fortran, C, Python	NAO, STO	Any	Yes	Yes	No	No	No	No	Yes, MAGMA
DFT++ (succeeded by JDFTx)	Free, GPL	C++	PW, Wavelet	3d	Yes	No	No	No	No	Yes	No
DIRAC	Academic	Fortran 77, Fortran 90, C	GTO	No	No	No	Yes	Yes	Yes	Yes	No
DMol3	Commercial	Fortran 90	NAO	Any	No	No	No	No	No	Yes	No
ELK	Free, GPL	Fortran 95	FP-LAPW	3d	No	No	Yes	No	No	Yes	No
Empire	Academic, commercial	Fortran	Minimal STO	Any	No	Yes	No	No	No	No	No
EPW[6]	Free, GPL	Fortran	PW	2d, 3d	No	No	No	No	No	Yes	No
ErgoSCF	Free, GPL	C++	GTO	No	No	No	Yes	No	No	Yes	No
ERKALE	Free, GPL	C++	GTO	No	No	No	Yes	No	No	Yes	No
Exabyte.io	Cloud, Free Tier	Python	PW	3d	Yes	Unknown	Unknown	Unknown	No	Yes	Yes
EXCITING	Free, GPL	Fortran 95	FP-LAPW	3d	No	No	Yes	No	No	Yes	No

FLEUR	Free, MIT	Fortran 95	FP-(L)APW+lo	1d, 2d, 3d	No	No	Yes	Yes	No	Yes	Yes
FHI-aims	Academic, commercial	Fortran	NAO	Any	Yes	No	Yes	Yes	No	Yes	Yes
FPLO[13]	Commercial	Fortran 95, C++, Perl	LO+minimum-basis, NAO	Any	No	No	No	No	No	Yes	No
FreeON (formely MondoSCF)	Free, GPL	Fortran 95	GTO	Any	Yes	No	Yes	Yes	No	Yes	No
Firefly (formely PC GAMESS)	Academic	Fortran, C, Assembly	GTO	No	Yes	Yes	Yes	Yes	Yes[16]	Yes	Yes
GAMESS (UK)	Academic (UK), commercial	Fortran	GTO	No	No	Yes	Yes	Yes	Yes	Yes	Yes
GAMESS (US)	Academic	Fortran	GTO	No	Yes[2]	Yes	Yes	Yes	Yes[16]	Yes	Yes
Gaussian	Commercial	Fortran	GTO	Any	Yes	Yes	Yes	Yes	No	Yes	Yes
GPAW	Free, GPL	Python, C	Grid, NAO, PW	Any	Yes	No	Yes[5]	No	No	Yes	Yes
HiLAPW	Unknown	Unknown	FLAPW	3d	No	No	No	No	No	Yes	No
HelFEM	Free, GPL	C++	Finite elements	No	No	No	Yes	No	No	Yes	No
HORTON	Free, GPL	Python, C++	GTO	No	No	No	Yes	Yes	No	Yes	No
HyperChem	Commercial	C++	STO, GTO	Yes	Yes	Yes	Yes	Yes	No	Yes	No
Jaguar	Commercial	Fortran, C	GTO	No	Yes	No[11]	Yes	Yes	No	Yes	No
JDFTx	Free, GPL	C++	PW	3d	No	No	Yes	No	No	Yes	Yes, CUDA
LOWDIN	Academic	Fortran 95, 03	GTO	No	Yes	No	Yes	Yes	No	Yes	No
MADNESS	Free, GPL	C++	Wavelet	No	No	No	Yes	Yes	No	Yes	No
Maple Quantum Chemistry Package	Commercial	Maple, C, Fortran, Python	GTO	No	No	No	Yes	Yes	No	Yes	No
MISSTEP	Free, GPL	C++	PW	No	No	No	No	No	No	Yes	No
MOLCAS	Academic, commercial[1][14]	Fortran, C, C++, Python, Perl	GTO	No	Yes	Yes	Yes	Yes	Yes	Yes	Yes
OpenMOLCAS	Free,[14] LGPL	Fortran, C, C++, Python, Perl	GTO	No	Yes	Yes	Yes	Yes	Yes	Yes	Yes
MolDS	Free, GPL	C++	STO, GTO	No	No	Yes	No	No	No	No	No
MOLGW	Free, GPL	Fortran	GTO	No	No	No	Yes	Yes	No	Yes	No
MOLPRO	Commercial	Fortran	GTO	No	No	No	Yes	Yes	Yes[17]	Yes	Yes
MONSTERGAUSS	Free	Fortran	GTO	No	No	No	Yes	Yes	No	No	No
MOPAC	Academic, commercial	Fortran	Minimal GTO	Any	No	Yes	No	No	No	No	Yes
MPQC	Free, LGPL	C++	GTO	No	No	No	Yes	Yes	No	Yes	No
MRCC	Academic	Fortran	GTO	No	Yes	No	Yes	Yes	Yes	Yes	No
NRLMOL	Unknown	Fortran	GTO	No	No	No	No	No	No	Yes	No
NTChem	Unknown	Unknown	GTO	No	No	No	Yes	Yes	No	Yes	No
NWChem	Free, ECL v2	Fortran 77, C	GTO, PW	Yes (PW), No (GTO)	Yes	No	Yes	Yes	No	Yes	Yes, CUDA
Octopus	Free, GPL	Fortran 95, C	Grid	Any	Yes	No	Yes	No	No	Yes	Yes, CUDA and OpenCL
ONETEP	Academic (UK), commercial	Fortran	PW	3d	Yes	No	Yes[5]	No	No	Yes	Yes, CUDA
OpenAtom	Academic	Charm++ (C++)	PW	3d	Yes	No	No	No	No	Yes	Yes
OpenMX	Free, GPL	C	NAO	3d	Yes	No	No	No	No	Yes	No
ORCA	Academic, commercial	C++	GTO	No	Yes	Yes	Yes	Yes	Yes[19]	Yes	No
phase0	Free, GPL		PW[2]	Unknown			Yes	No	No	Yes	No
PLATO	Academic	Unknown	NAO	Any	Yes	No	No	No	No	Yes	No
PQS	Commercial	Unknown	Unknown	Unknown	Yes	Yes	Yes	Yes	No	Yes	No

Priroda (see also [1])	Academic	C	GTO	No	No	Yes	Yes	Yes	No	Yes	No
PSI	Free, GPL	C, C++, Python	GTO	No	No	No	Yes	Yes	Yes	Yes	No
PUPIL	Free, GPL	Fortran, C	GTO, PW	Any	Yes	Yes	Yes	Yes	No	Yes	Yes
PWmat	Commercial	Fortran	PW	3d	Yes	No	Yes	Yes	No	Yes	Yes
PWscf[6]	Free, GPL	Fortran	PW	3d	No	No	Yes	No	No	Yes	No
PyQuante	Free, BSD	Python	GTO	No	No	Yes	Yes	Yes	No	Yes	No
PySCF	Free, BSD	Python	GTO	Yes	No	No	Yes	Yes	No	Yes	No
Qbox	Free, GPL	C++	PW	3d	Yes	No	Yes	No	No	Yes	No
Q-Chem	Academic, commercial	Fortran, C, C++	GTO	No	Yes	Yes	Yes	Yes	No	Yes	Yes
QMCPACK (QMC)	Free, U. Illinois Open Source	C++	GTO, PW, Spline, Grid, STO	Any	No	No	Yes	Yes	Yes[18]	No	Yes, CUDA
Quantemol-N	Academic, commercial	Fortran	GTO	No	Yes	Yes	Yes	Yes	No	No	No
QSite	Unknown	Unknown	GTO	No	Yes	No[11]	Yes	Yes	No	Yes	No
Quantum ESPRESSO	Free, GPL	Fortran	PW	3d	Yes	No	Yes	No	No	Yes	Yes, CUDA
RMG	Free, GPL	C, C++	Grid	Any	Yes	No	No	No	No	Yes	Yes, CUDA
RSPt	Academic	Fortran, C	FP-LMTO	3d	No	No	No	No	No	Yes	Yes
SAMSON	Free	C++, Python	Multiple	No	Yes	Yes	No	No	No	Yes	No
Scigress	Commercial	C++, C, Java, Fortran	GTO	Yes	Yes	Yes	No	No	No	Yes	No
Siam Quantum	Free, GPL	C	GTO	No	Yes	No	Yes	Yes	No	Yes	No
SIESTA	Free, GPL	Fortran	NAO	3d[12]	Yes	No	No	No	No	Yes	No
Spartan	Commercial	Fortran, C, C++	GTO	No	Yes	Yes	Yes	Yes	No	Yes	No
SPHInX	Free, Apache License	C++	PW	3d	No	No	No	No	No	Yes	No
TB-LMTO	Academic	Fortran	LMTO	3d	No	No	No	No	No	Yes	No
TeraChem [8]	Commercial	C, CUDA	GTO	No	Yes	No	Yes	Yes	No	Yes	Yes
TURBOMOLE	Commercial	Fortran	GTO	Yes	Yes	No	Yes	Yes	No	Yes	No
VASP	Academic (AT), commercial	Fortran	PW	3d	Yes	No	Yes	Yes	No	Yes	Yes
WIEN2k	Commercial	Fortran, C	FP-(L)APW+lo	3d	Yes	No	Yes	No	No	Yes	No
xtb	Academic	Fortran	Minimal GTO	3d	No	Yes	No	No	No	No	No
Yambo Code	Free, GPL	Fortran	PW	3d	No	No	Yes	Yes	No	No	No
Package	**License**†	**Language**	**Basis**	**Periodic**‡	**Mol. mech.**	**Semi-emp.**	**HF**	**Post-HF**	**MRCI**	**DFT**	**GPU**

Post processing packages in quantum chemistry and solid-state physics [edit]

Package	License†	Language	Input	what it calculate
wannier90	Free, GPL	Fortran	interfaces with some DFT packages	Maximally-Localised Wannier Functions,Density of States, Berry phase properties including, Transport

footnotes [edit]

† "Academic": academic (no cost) license possible upon request; "Commercial": commercially distributed.

‡ Support for periodic systems (3d-crystals, 2d-slabs, 1d-rods and isolated molecules): 3d-periodic codes always allow simulating systems with lower dimensionality within a supercell. Specified here is the ability for simulating within lower periodicity.

[1] The CAMPOS project(which includes Dacapo) states that all code is GPL. The Dacapo distribution contains no license information.

[2] QuanPol is a full spectrum and seamless (HF, MCSCF, GVB, MP2, DFT, TDDFT, CHARMM, AMBER, OPLSAA) QM/MM package integrated in GAMESS-US.[3]

[3] Through Ascalaph

[4] Through interface to MOPAC

[5] Using exact exchange DFT

[6] Distributed with Quantum ESPRESSO

[7] Web service integrating MPQC.

[8] TeraChem is the first fully GPU-accelerated quantum chemistry software.

[9] Atomistix ToolKit also contains finite-bias NEGF electron transport calculations with open boundary conditions.

[10] Through CRYSCOR program.

[11] However, available in the Schrödinger Suite.

[12] SIESTA also contains finite-bias NEGF electron transport calculations with open boundary conditions using TranSIESTA.

[13] FPLO has fully relativistic calculation.

[14] In September 2017, large part of MOLCAS was released under LGPL.

[15] Gamma point only.

[16] Supports MRCI calculations only in the FOCI (first order CI) and SOCI (second order CI) variants.

[17] Supports MRCI calculations only in internally-contracted forms (two variants are possible).

[18] Supports MRCI-type calculations though general selected-CI.

[19] Supports both full, uncontracted MRCI and contracted MRCI using two contraction schemes.

Further programs [edit]

- AIMPRO
- Ascalaph Designer
- PWPAW, Atompaw
- Deneb
- Fireball
- FSatom
- MAPS
- Newton-X
- NRLMOL
- ParaGauss
- PARATEC
- PARSEC
- Petot
- QMCPACK
- Socorro
- S/PHI/nX
- SPR-KKR

See also [edit]

- List of software for Monte Carlo molecular modeling
- Comparison of software for molecular mechanics modeling
- Molecular design software
- Molecule editor
- Molecular modeling on GPUs
- List of software for nanostructures modeling
- Semi-empirical quantum chemistry methods
- Computational chemical methods in solid state physics, with periodic boundary conditions
- Valence bond programs
- Car–Parrinello molecular dynamics

References [edit]

1. ^ "Order MOLCAS".
2. ^ Kaneko, Tomoaki; Tajima, Nobuo; Yamasaki, Takahiro; Nara, Jun; Schimizu, Tatsuo; Kato, Koichi; Ohno, Takahisa (2018). "Hybrid density functional analysis of distribution of carbon-related defect levels at 4H-SiC(0001)/SiO2 interface". *Applied Physics Express*. **11** (1): 011302. Bibcode:2018APExp..11a1302K. doi:10.7567/APEX.11.011302. ISSN 1882-0778.
3. ^ Change History of GAMESS

Further reading [edit]

- Young, David (2001). *Computational Chemistry: A Practical Guide for Applying Techniques to Real World Problems*. New York: John Wiley & Sons. pp. 322–359. ISBN 978-0-471-33368-5.
- "NVIDIA GPU Applications". NVIDIA. Retrieved 9 July 2014.
- "Major codes in electronic-structure theory, quantum chemistry, and molecular-dynamics - Nomad repository". NOMAD. Retrieved 19 November 2017.

v · t · e	Computational chemistry software	[hide]
Cheminformatics	Open-source	Avalon Cheminformatics Toolkit · Bioclipse · Blue Obelisk · Chemistry Development Kit · ECCE · JOELib · OELib · Open Babel · RDKit
	Proprietary	Canvas · Chemicalize · Discovery Studio
Chemical kinetics	Open-source	APBS · Cantera · KPP
	Proprietary	Autochem · Chemical WorkBench · CHEMKIN · COSILAB · DelPhi · Khimera
Molecular modelling and visualization	List of molecular graphics systems	
	Open-source	Ascalaph Designer · Avogadro · BALL · Biskit · CPMD · Gabedit · Ghemical · Jmol · Molekel · PyMOL · QuteMol · RasMol
	Proprietary	Abalone · ACD/ChemSketch · Atomistix ToolKit · ChemDraw · EzMol · Gaussian · Maestro · MarvinSketch · MarvinView · MODELLER · Molecular Operating Environment · Spartan · UCSF Chimera · VMD
Molecular docking	List of protein-ligand docking software	
	Open-source	AutoDock · AutoDock Vina · FlexAID · rDock
	Proprietary	Glide · LeDock · Molecular Operating Environment

Molecular dynamics	**Open-source**	GROMACS · LAMMPS · OpenMM · PLUMED
	Proprietary	Abalone · AMBER · CHARMM · Desmond · GROMOS · NAMD
Quantum chemistry	**List of quantum chemistry and solid-state physics software**	
	Open-source	ABINIT · ACES (CFOUR) · AIMAll · BigDFT · CP2K · DACAPO · Dalton · DP code · FreeON · HORTON · MADNESS · MPQC · NWChem · Octopus · PSI · PyQuante · PySCF · Quantum ESPRESSO (PWscf) · RMG · SAMSON · SIESTA · VB2000 · YAMBO code
	Proprietary	ADF · AMPAC · DMol3 · CADPAC · CASINO · CASTEP · COLUMBUS · CONQUEST · CPMD · CRUNCH · CRYSTAL · DIRAC · Firefly · GAMESS (UK) · GAMESS (US) · Gaussian · Jaguar · MOLCAS · MOLPRO · MOPAC · ONETEP · OpenAtom · ORCA · PARSEC · PLATO · PQS · Q-Chem · Quantemol · Scigress · Spartan · TeraChem · TURBOMOLE · VASP · WIEN2k · XMVB
Skeletal structure drawing	**Open-source**	BKChem · JChemPaint · JME Molecule Editor · Molsketch · XDrawChem
	Proprietary	ACD/ChemSketch · ChemDoodle · ChemDraw · MarvinSketch
Others		Aqion · Eulim · EXC code · GenX · GSim · ICM (ICM-Browser) · Materials Studio · Molden · OpenChrom · RubyChem · SASHIMI

Categories: Density functional theory software | Computational chemistry software | Molecular modelling software | Physics software | Lists of software

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