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 the capabilities of the most versatile software packages that show an entry in two or more columns of the table.

Package	License†	Lang.	Basis	Periodic‡	Mol. mech.	Semi-emp.	HF	Post-HF	DFT
ABINIT	GPL	Fortran	PW	3d	Yes	No	No	No	Yes
ACES II	GPL	Fortran	GTO	No	No	No	Yes	Yes	Yes
ACES III	GPL	Fortran/C++	GTO	No	No	No	Yes	Yes	No
ADF	Commercial	Fortran	STO	Any	Yes	Yes[4]	Yes	No	Yes
Atomistix ToolKit (ATK)	Commercial	C++/Python	NAO/EHT	3d[9]	Yes	Yes	No	No	Yes
BigDFT	GPL	Fortran	Wavelet	Any	Yes	No	Yes	No	Yes
CADPAC	Academic	Fortran	GTO	No	No	No	Yes	Yes	Yes
CASINO (QMC)	Academic	Fortran 95	GTO / PW / Spline / Grid / STO	Any	No	No	Yes	Yes	No
CASTEP	Academic (UK) / Commercial	Fortran	PW	3d	Yes	No	Yes[5]	Yes	Yes
CFOUR	Academic	Fortran	GTO	No	No	No	Yes	Yes	No
COLUMBUS	Academic	Fortran	GTO	No	No	No	Yes	Yes	No
CONQUEST	Academic	Fortran 90	NAO/Spline	3d	Yes	No	Yes[5]	No	Yes
CP2K	GPL	Fortran 95	Hybrid GTO / PW	3d	Yes	Yes	Yes	Yes	Yes
CPMD	Academic	Fortran	PW	3d	Yes	No	Yes	No	Yes
CRYSTAL	Academic (UK) / Commercial	Fortran	GTO	Any	Yes	No	Yes	Yes[10]	Yes
DACAPO	GPL ?[1]	Fortran	PW	3d	Yes	No	No	No	Yes
DALTON	Academic	Fortran	GTO	No	No	No	Yes	Yes	Yes
DFTB+ (http://www.dftb-plus.info)	Academic / Commercial	Fortran 95	NAO	Any	Yes	Yes	No	No	No
DFT++ (http://dft.physics.cornell.edu/)	GPL	C++	PW / Wavelet	3d	Yes	No	No	No	Yes
DIRAC	Academic	Fortran 77, Fortran 90, C	GTO	No	No	No	Yes	Yes	Yes
DMol3	Commercial	Fortran 90	NAO	Any	No	No	No	No	Yes
ELK	GPL	Fortran 95	FP-LAPW	3d	No	No	Yes	No	Yes
ErgoSCF (http://www.ergoscf.org)	GPL	C++	GTO	No	No	No	Yes	No	Yes
ERKALE (http://erkale.googlecode.com)	GPL	C++	GTO	No	No	No	Yes	No	Yes
EXCITING	GPL	Fortran 95	FP-LAPW	3d	No	No	Yes	No	Yes
FLEUR (http://www.flapw.de)	Academic	Fortran 95	FP-(L)APW+lo	3d, 2d, 1d	No	No	Yes	Yes	Yes
FHI-aims (http://www.fhi-berlin.mpg.de/aims/)	Commercial	Fortran	NAO	Any	Yes	No	Yes	Yes	Yes
FreeON	GPL	Fortran 95	GTO	Any	Yes	No	Yes	Yes	Yes
Firefly / PC GAMESS	Academic	FORTRAN, C, Assembly	GTO	No	Yes[3]	Yes	Yes	Yes	Yes
GAMESS (UK)	Academic (UK) / Commercial	Fortran	GTO	No	No	Yes	Yes	Yes	Yes
GAMESS (US)	Academic	Fortran	GTO	No	Yes[2]	Yes	Yes	Yes	Yes

Gaussian	Commercial	Fortran	GTO	Any	Yes	Yes	Yes	Yes	Yes
GPAW (https://wiki.fysik.dtu.dk/gpaw/)	GPL	Python / C	Grid / NAO / PW	3d	Yes	No	Yes[5]	No	Yes
HiLAPW (http://home.hiroshima-u.ac.jp/fpc/manuals/HiLAPW/HiLAPW.html)	Unknown	Unknown	FLAPW	3d	No	No	No	No	Yes
Jaguar	Commercial	Fortran / C	GTO	No	Yes	No[11]	Yes	Yes	Yes
JDFTx (http://jdftx.sourceforge.net/)	GPL	C++ / CUDA	PW	3d	No	No	Yes	No	Yes
MADNESS	GPL	C++	Wavelet	No	No	No	Yes	No	Yes
MISSTEP	GPL	C++	PW	No	No	No	No	No	Yes
MOLCAS	Commercial	Fortran	GTO	No	Yes	Yes	Yes	Yes	Yes
MolDS (http://en.sourceforge.jp/projects/molds/)	GPL	C++	STO/GTO	No	No	Yes	No	No	No
MOLPRO	Commercial	Fortran	GTO	No	No	No	Yes	Yes	Yes
MOPAC	Academic / Commercial	Fortran	Minimal GTO	Any	No	Yes	No	No	No
MPQC	LGPL	C++	GTO	No	No	No	Yes	Yes	Yes
NRLMOL (http://quantum.utep.edu/nrlmol/nrlmol.html)	Unknown	Fortran	GTO	No	No	No	No	No	Yes
NTChem (http://labs.aics.riken.jp/nakajimat_top/ntchem_e.html)	Unknown	Unknown	GTO	No	No	No	Yes	Yes	Yes
NWChem	ECL v2	Fortran 77 / C	GTO, PW	Yes(PW) No(GTO)	Yes	No	Yes	Yes	Yes
Octopus	GPL	Fortran 95, C, OpenCL	Grid	Any	Yes	No	Yes	No	Yes
ONETEP	Academic (UK) / Commercial	Fortran	PW	3d	Yes	No	Yes[5]	No	Yes
OpenAtom	Academic	Charm++ (C++)	PW	Template:3d	Yes	No	No	No	Yes
OpenMX (http://www.openmx-square.org/)	GPL	C	NAO	3d	Yes	No	No	No	Yes
ORCA	Academic	C++	GTO	No	Yes	Yes	Yes	Yes	Yes
PLATO	Academic	Unknown	NAO	Any	Yes	No	No	No	Yes
PQS	Commercial	Unknown	Unknown	Unknown	Yes	Yes	Yes	Yes	Yes
Priroda-06 (http://www.physto.se/~laikov/p/)	Academic	C	GTO	No	No	No	Yes	Yes	Yes
PSI	GPL	C / C++	GTO	No	No	No	Yes	Yes	Yes
PWscf[6]	GPL	Fortran	PW	3d	No	No	Yes	No	Yes
PyQuante	BSD	Python	GTO	No	No	Yes	Yes	Yes	Yes
Q-Chem	Commercial	Fortran / C++	GTO	No	Yes	Yes	Yes	Yes	Yes
Quantemol-N	Academic / Commercial	Fortran	GTO	No	Yes	Yes	Yes	Yes	No
Quantum ESPRESSO	GPL	Fortran	PW	3d	Yes	No	Yes	No	Yes
RSPt (http://www.rspt.net)	Academic	Fortran / C	FP-LMTO	3d	No	No	No	No	Yes
SCIGRESS	Commercial	C++, C, Java, Fortran	GTO	Yes	Yes	Yes	No	No	Yes
Spartan	Commercial	Fortran / C / C++	GTO	No	Yes	Yes	Yes	Yes	Yes
Siam Quantum (http://www.physics.kku.ac.th/sq)	GPL	C	GTO	No	No	No	Yes	Yes	No
SIESTA	Academic	Fortran	NAO	3d	Yes	No	No	No	Yes
TB-LMTO (http://www.fkf.mpg.de/andersen/)	Academic	Fortran	LMTO	3d	No	No	No	No	Yes
TERACHEM [8]	Commercial	C/CUDA	GTO	No	Yes	No	Yes	No	Yes
TURBOMOLE	Commercial	Fortran	GTO	No	Yes	No	Yes	Yes	Yes
VASP	Academic(AT)/ Commercial	Fortran	PW	3d	Yes	No	Yes	Yes	Yes
WIEN2k	Commercial	Fortran / C	FP-(L)APW+lo	3d	Yes	No	Yes	No	Yes
Yambo Code	GPL	Fortran	PW	3d	No	No	Yes	Yes	No

† “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 the simulation of systems with lower dimensionality within a supercell. Specified here is the capability for actual simulation within lower periodicity.

[1] The CAMPOS project (http://www.camd.dtu.dk/software.aspx) (which includes Dacapo) states that all code is GPL. The Dacapo distribution itself does not contain any 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.[1]

[3] Through Ascalaph (http://www.biomolecular-modeling.com/Products.html)

[4] Through interface to MOPAC

[5] Using exact exchange DFT

[6] Distributed with Quantum ESPRESSO (http://www.quantum-espresso.org)

[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 (http://www.cryscor.unito.it) program.

[11] However, available in the Schrödinger Suite.

Further programs

- AIMPRO (http://aimpro.ncl.ac.uk/)
- Ascalaph Designer
- PWPAW / Atompaw
- Deneb (http://www.atelgraphics.com)
- deMon2K (http://www.demon-software.com/public_html/program.html)
- DFTB+ (http://www.dftb-plus.info/)
- Fireball (http://www.fireball-dft.org)
- FSatom (http://www.tddft.org/fsatom)
- MAPS (http://www.scienomics.com/products/molecular-modeling-platform)
- NRLMOL (http://quantum.utep.edu/nrlmol/nrlmol.html)
- ParaGauss (http://qcl.theochem.tu-muenchen.de/ParaGauss.html)
- PARATEC
- PARSEC
- Petot (http://hpcrd.lbl.gov/~linwang/PEtot/PEtot.html)
- QMCPACK (http://qmcpack.cmscc.org)
- Socorro (http://dft.sandia.gov/Socorro/mainpage.html)
- S/PHI/nX (http://www.sphinxlib.de)
- SPR-KKR (http://olymp.cup.uni-muenchen.de/ak/ebert/SPRKKR)

See also

- List of software for Monte Carlo molecular modeling
- Molecular mechanics programs
- Molecular design software
- Molecule editor
- Molecular modeling on GPU
- Nanostructures modeling programs
- Semi-empirical programs
- Solid state system programs with periodic boundary conditions.
- Valence bond programs

References

1. **^** Change History of GAMESS (http://www.msg.ameslab.gov/gamess/versions.html)

- Young, David (2001). *Computational Chemistry: A Practical Guide for Applying Techniques to Real World Problems*. New York: John Wiley & Sons. pp. 322–359. ISBN 0-471-33368-9.