

# Jaguar

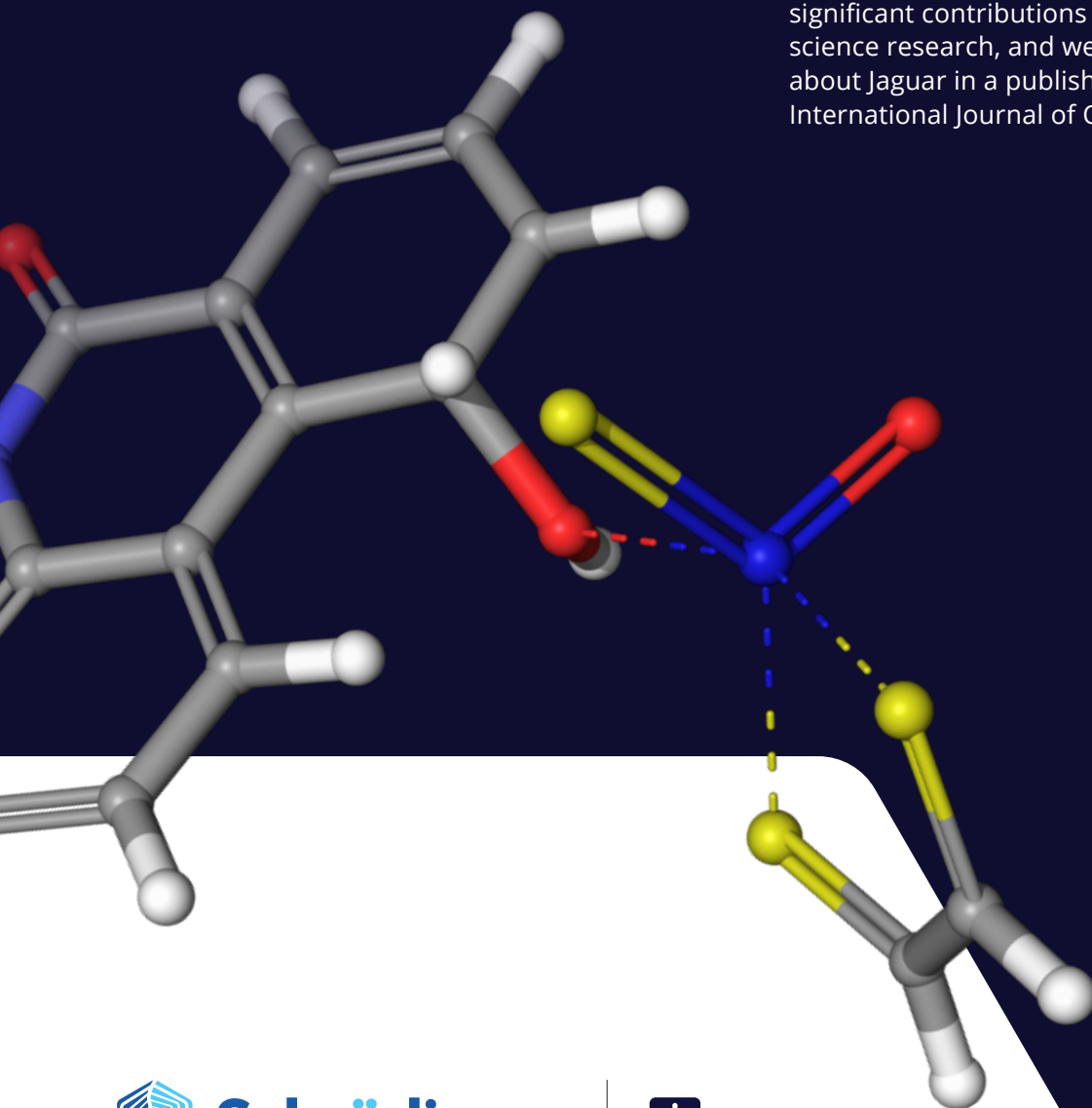
Ever since its inception, Jaguar was designed with one goal in mind — to help researchers solve practical, real-world problems. To meet this goal, Jaguar's development has focused on performance and scientific accuracy. Furthermore, Jaguar is easy to use — with a world-class graphical interface and automated workflows that guide new users through complex *ab initio* quantum mechanics (QM) analyses for a vast range of chemical systems. Jaguar is fully integrated into Schrödinger's suites of scientific solutions, making interoperability with other programs seamless.

## Key Advantages

Jaguar specializes in fast electronic structure predictions for molecular systems of medium and large size via the use of the pseudospectral (PS) method<sup>1</sup> and computational strategies that scale reasonably as system size grows, in particular density functional theory (DFT). Jaguar supports parallel computation through OpenMP to further take advantage of modern hardware improvements.

Significant ongoing efforts have been devoted to improving the accuracy of predictions including the transition metal initial guess wavefunction algorithm, recent advances in  $pK_a$  predictions, and enabling access to machine learning potentials (MLP).

Schrödinger has devoted and continues to devote development resources to enhance Jaguar's feature set and to improve Jaguar's robustness and performance. To date, Jaguar has made significant contributions in both life and materials science research, and we invite you to learn more about Jaguar in a published review article in the International Journal of Quantum Chemistry.<sup>2</sup>

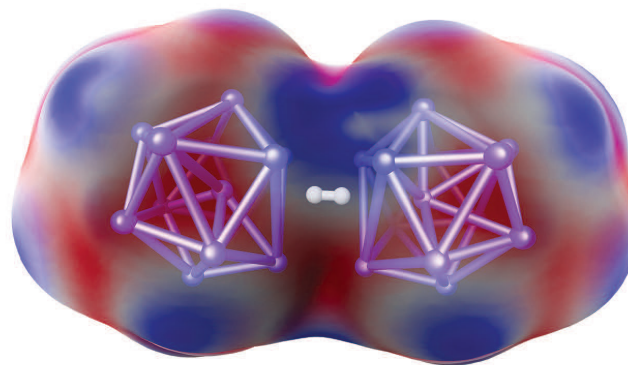


# Jaguar for Materials Science

Jaguar is a powerful tool for studying the chemical reactions and properties that are implicated in the assembly, operation or failure of materials, or for the discovery and optimization of new materials solutions. Jaguar's speed and accuracy make it an efficient and robust tool for the routine treatment of realistic chemical models.

An exciting application of Jaguar is for the *ab initio* design or high throughput virtual screening for new materials with novel or enhanced properties — made possible by taking advantage of Jaguar's industry-leading efficiency and robustness and Schrödinger Materials Science Suite's combinatorial chemistry solutions to rapidly enumerate compound libraries.

Below are some example applications of Jaguar for a diverse range of technologically important chemical systems.



Cluster-based materials are being investigated for a variety of materials applications. Here the electronic charge distribution at the dimer is shown mapped onto the electron density. An  $H_2$  molecule is shown trapped within the dimer.

## Molecular Catalysis

Jaguar has been used extensively to provide insight to enable the rational design of improved catalysts. Geometric effects and orbital/electrostatic interactions that provide the basis for catalyst stability, selectivity, and activity are difficult or impossible to gain by experiment alone, but can be efficiently computed and analyzed using Jaguar.

## Optoelectronics and Photovoltaics

Molecular properties such as electronic energies, multipole moments, linear and higher order polarizabilities, ionization and reduction potentials, and charge reorganization energies can be evaluated computationally to aid in the selection or design of organic optoelectronic materials. Jaguar has been used to analyze a variety of organic semiconductors including derivatized oligothiophenes, cyanated tetracenes, and N-heteropentacenes, and other materials for dye sensitized solar cells (DSSC).

## Molecular Electronics

Jaguar has been used to investigate the mechanism of carbon nanotube growth, the conformation dependence of molecular conduction, the electronic structure of molecular rectifiers, switching in mechanically interlocked molecules, and interference effects in conduction through arene molecular wires.

## Energy Capture and Storage

First-principles simulations using Jaguar have been used to analyze the chemical mechanisms and controlling energetics for the operation and failure modes for candidate energy storage materials such as Li-air batteries.

## Thin Film Processing

The geometric and electronic structure of organometallic precursor chemicals can be rapidly and efficiently computed with Jaguar, so as to quantify their gas-phase thermal stability, dimerization and reactivity at surfaces during thin film deposition or etch. Complementing this are tools for easily building organometallic complexes and establishing their spin state.

# Product Details

## Automated Workflows for Advanced Analyses

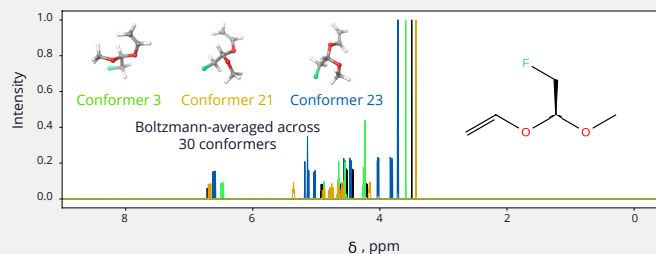
- Counterpoise calculations
- $pK_a$  prediction (through separate Jaguar  $pK_a$  and Macro- $pK_a$  modules)
- Automated transition state search (through a separate AutoTS module)<sup>3</sup>
- Intermolecular hydrogen bond binding energy
- Fukui functions calculations
- Heat of formation
- Conformationally averaged IR/VCD, UV-vis/ECD, and NMR spectra calculations (available through Jaguar Spectroscopy module)
- $\Delta E$ ,  $\Delta H$ ,  $\Delta G$  of a chemical reaction
- Conformer and tautomer predictor
- Estimated computational time through machine learning

## Molecular Properties

- Electrostatic potential (ESP) surface and analysis
- Average local ionization energy (ALIE) surface
- Electron density and spin density surfaces
- Dipole, quadrupole, octupole, and hexadecapole moments
- Analytic static polarizabilities, first and second hyperpolarizabilities
- Analytic dynamic (frequency-dependent) polarizabilities and hyperpolarizabilities
- Fukui functions and atomic indices
- Visualized noncovalent interactions
- Natural bond orbital (NBO) analysis through the built-in third-party NBO 7.0 package
- Harmonic and anharmonic vibrational frequencies
- Mulliken population analysis
- Mulliken, ESP, and Stockholder charges
- Thermochemical properties: constant volume heat capacity, internal energy, enthalpy, entropy, Gibbs free energy at varying temperatures and pressures, heat of formation
- Ab initio  $pK_a$  prediction (through separate Jaguar  $pK_a$  and Macro- $pK_a$  modules)
- Excited states through CIS, TDDFT, and  $\Delta$ SCF theories

## Geometry Optimization

- Geometry optimizations for equilibrium structures and transition states, in gas phase and solution
- Geometry optimizations of excited states with TDDFT
- Cartesian, redundant, and internal coordinates
- Constraints on bond lengths, bond angles, torsional angles
- Constraints on Cartesian or internal coordinates, frozen or harmonic
- Standard, linear synchronous transit (LST), and quadratic synchronous transit (QST) transition state optimizations
- Fischer-Almlöf, Schlegel, user-supplied, and quantum-mechanical Hessian guesses; BFGS, Powell, and Murtagh-Sargent/Powell Hessian updates
- Intrinsic reaction coordinate (IRC) scans
- Rigid, relaxed, and dynamic coordinate scans
- Post-convergence analysis
- Prevent chemical reactions during geometry optimizations
- Automatically detect and move away from saddle points



A DFT-simulated, Boltzmann-averaged  $^1\text{H}$  NMR spectrum of an organic molecule in chloroform together with the spectra of some of its individual conformers.

## Solvation

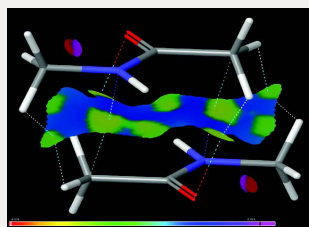
- Poisson-Boltzmann finite-element (PBF) self-consistent reaction field (SCRF), energies and geometry optimizations
- van der Waals radii- and isodensity-based PBF
- Several versions of polarizable continuum model (PCM), energies and geometry optimizations
- SM6 and SM8 energies
- Support for multiple solvents
- Generation of COSMOtherm input files (.cosmo files)

## Spectroscopy

- Infrared (IR) intensities
- Vibrational circular dichroism (VCD) spectra
- Electronic circular dichroism (ECD) spectra
- NMR shielding constants and spin-spin coupling constants in gas phase and solution
- $^1\text{H}$  and  $^{13}\text{C}$  NMR chemical shifts
- UV-vis spectra through CIS or TDDFT calculations
- Visualizing conformationally-averaged IR, UV-vis, VCD, ECD, and NMR spectra through Maestro
- Automated alignment of theoretical and experimental IR/VCD spectra in Maestro
- Raman intensities
- Mössbauer isomer shifts and quadrupole splittings for  $^{57}\text{Fe}$  and other isotopes

## Parallel

- Analytic and pseudospectral calculations
- HF and DFT energies
- HF and DFT geometry optimizations
- HF and DFT second derivatives (vibrational frequencies)
- HF and DFT VCD spectra
- Closed-shell LMP2 and RI-MP2 calculations
- CIS and TDDFT energies
- NMR shielding constants and spin-spin couplings
- Polarizabilities and hyperpolarizabilities
- SM6 and SM8 solvation models



An NCI plot for the equilibrium geometry of N-methylacetamide dimer. Weak internal C – H O hydrogen bonds are indicated as disks of purple and red, whereas the intermolecular bonding is indicated by the yellow-greenish regions, in which there are bond critical points in the density.

## Levels of Theory

### Density Functional Theory (DFT)

- Exchange functionals: HFS, Xalpha, Becke 88, PW91, Barone-modified PW91, OPTX
- Correlation functionals: VWN, VWN5, LYP, P86, PW91, B95, Perdew-Zunger 81, PBE, HCTH407
- GGA functionals: SOGGA, SOGGA11, HCTH407, GAM, N12, BOP, GLYP, KT2, rPBE, revPBE
- Meta-GGA functionals: TPSS, revTPSS, SCAN, r2SCAN, NPKZB, MGGA-MS0, MGGA-MS1, MGGA-MS2
- Hybrid functionals: B3LYP, O3LYP, X3LYP, B3P86, B3PW91, B97-1, B98, SB98, PBE0, PWB6K, PW6B95, MPW1K, MPWB1K, MPW1PW91, BB1K, BHandH, BHandHLYP, M05, M05-2X, M06, M06-2X, M06-L, M06-HF, PBE, B3LYP-LOC, M08-HX, M08-SO, MN12-L, MN15-L, and MN15,  $\omega$ B97X-D3,  $\omega$ B97X-D3(BJ),  $\omega$ B97X-V,  $\omega$ B97M-V, TPSSh, revTPSSh, SOGGA11-X, SCAN0, MGGA-MS2h, MN12-SX
- Dispersion-corrected functionals: B97-D, B3LYP-D3, B3PW91-D3, MPWB1K-D3, M05-D3, M05-2X-D3, M06-D3, M06-HF-D3, M06-2X-D3, PBE0-D3, B1B95-D3, BP86-D3, BLYP-D3, OLYP-D3, PBE-D3, B97-D3, B3LYP-MM, PBE-ulg, CAM-B3LYP-D3,  $\omega$ PBE-D3, B3LYP-D3(BJ), B3PW91-D3(BJ), PW6B95-D3(BJ), PBE0-D3(BJ), B1B95-D3(BJ), BP86-D3(BJ), BLYP-D3(BJ), OLYP-D3(BJ), PBE-D3(BJ), B97-D3(BJ), CAM-B3LYP-D3(BJ),  $\omega$ PBE-D3(BJ),  $\omega$ B97X-D3,  $\omega$ B97X-D3(BJ) and their D4-analogs
- Long range-corrected functionals: CAM-B3LYP, LRC-BLYP, uPBE, uPBE0,  $\omega$ PBE,  $\omega$ PBEh, HSE03, HSE06, M11, M11-L,  $\omega$ B97,  $\omega$ B97x, BNL, CAM-B3LYP-D3,  $\omega$ PBE-D3,  $\omega$ PBE-D3(BJ),  $\omega$ B97X-D3,  $\omega$ B97X-D3(BJ), MN12-SX,  $\omega$ B97X-V,  $\omega$ B97M-V
- Dispersion-corrected long-range corrected functionals: CAM-B3LYP-D3,  $\omega$ PBE-D3,  $\omega$ B97X-D
- 3c composite methods: HF-3c, PBEh-3c, B97-3c, r2SCAN-3c,  $\omega$ B97X-3c

### Basis Sets

- Gaussian-type orbitals (GTO); s-, p-, d-, f-, and g-functions with up to 2<sup>nd</sup> derivatives
- Analytic STO-3G, 3-21G, 4-21G, 4-31G, 6-21G, 6-31G, 6-311G(3df, 3pd), 6-31G(TM), D95, D95V, MSV, (aug-)cc-pV[D,T,Q]Z, d-aug-cc-pv[D,T]Z, t-aug-cc-pv[D,T]Z, (aug-)cc-pVQZ-pp, MIDIX, TZV, def2-svp, def2-svpd, def2-tzvp, def2-tzvpd, def2-tzvpd, def2-qzvp, def2-qzvpd, def2-qzvpd, def2-qzvpd, NLO-V, ANO-VT, PolX
- Pseudospectral 3-21G, 6-31G, 6-311G, 6-31G(TM), D95, (aug-)cc-pV[D,T,Q]Z, (aug-)cc-pVTZ-PP, MIDIX, def2-svpd, def2-tzvp, and def2-tzvpd families
- Effective core potential (ECP) LAV1S, LAV2D, LAV2P, LAV3D, LAV3P, LACVD, LACVP, LACV3P, cc-pVTZ-pp, CSDZ, ERMLER2, LANL2DZ, LANL2TZ
- Relativistic sarc-zora, dyall-v2z\_zora-j-pt-gen, and dyall-2zcvp\_zora-j-pt-gen
- Diffuse and/or polarization functions are available for most basis sets
- Custom basis set and automatic conversion from Gaussian to Jaguar format
- Automated counterpoise calculations

- Restricted (RHF), unrestricted (UHF), and spin-restricted (ROHF) wave functions
- Energies and gradients are available for all, and second derivatives for the vast majority of the functionals (including D3- and D4-corrected)
- $\Delta$ SCF theory compatible with most density functionals

### Hartree-Fock (HF)

- RHF, UHF, and ROHF wave functions
- Energies, gradients, and second derivatives

### Møller-Plesset Perturbation Theory

- Local MP2 (LMP2) based on RHF and ROHF wave functions
- LMP2 energies, gradients, and numerical second derivatives
- Resolution of identity MP2 (RI-MP2) energies and gradients

### Time-Dependent Density Functional Theory (TDDFT) and Configuration Interaction Singles (CIS)

- RHF wave functions
- Energies, gradients, and second derivatives

### Zeroth Order Regular Approximation (ZORA)

- Energies
- Scalar and spin-orbit Hamiltonians
- Can be combined with TDDFT

### Other

- Third-party GFN2-xTB semiempirical theory
- Machine learning potential QRNN<sup>4</sup>

## References

1. R. A. Friesner, R. B. Murphy, M. D. Beachy, M. N. Ringnalda, W. T. Pollard, B. D. Dunietz, Y. Cao, *J. Phys. Chem. A*, 1999, 103, 1913.
2. A. D. Bochevarov, E. Harder, T. F. Hughes, J. R. Greenwood, D. A. Braden, D. M. Philipp, D. Rinaldo, M. D. Halls, J. Zhang, R. A. Friesner, *Int. J. Quantum Chem.*, 2013, 113, 2110.
3. L. D. Jacobson, A. D. Bochevarov, M. A. Watson, T. F. Hughes, D. Rinaldo, S. Ehrlich, T. B. Steinbrecher, S. Vaitheeswaran, D. M. Philipp, M. D. Halls, R. A. Friesner, *J. Chem. Theory Comput.* 2017, 13, 11, 5780–5797.
4. L. D. Jacobson, J. M. Stevenson, F. Ramezanghorbani, D. Ghoreishi, K. Leswing, E. D. Harder, R. Abel, *J. Chem. Theory Comput.* 2022, 18, 4, 2354–2366.

Contact us: [sales@schrodinger.com](mailto:sales@schrodinger.com)

Learn more: [www.schrodinger.com](http://www.schrodinger.com)



Schrödinger



Materials