Resource Summary Report

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Gamess

RRID:SCR_014896
Type: Tool

Proper Citation

Gamess (RRID:SCR_014896)

Resource Information

URL: http://www.msg.chem.iastate.edu/gamess/

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Description: Software program for ab initio molecular quantum chemistry. GAMESS can compute SCF wavefunctions ranging from RHF, ROHF, UHF, GVB, and MCSCF. Capabilities include using nuclear gradients for automatic geometry optimization, modeling of solvent effects, computation of the energy hessian for prediction of vibrational frequencies, as well as computation of nuclear wavefunctions. The program can also compute variety of molecular properties, ranging from simple dipole moments to frequency dependent hyperpolarizabilities.

Synonyms: The General Atomic and Molecular Electronic Structure System

Resource Type: source code, software resource

Keywords: molecular quantum chemistry, molecular properties, computation, analysis, visualization

Resource Name: Gamess

Resource ID: SCR_014896

License URLs: http://www.msg.chem.iastate.edu/gamess/License_Agreement.html

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Record Last Update: 20260729T044337+0000

Ratings and Alerts

No rating or validation information has been found for Gamess.

No alerts have been found for Gamess.

Data and Source Information

Source: SciCrunch Registry

Usage and Citation Metrics

We found 263 mentions in open access literature.

Listed below are recent publications. The full list is available at nidm-terms .

Azamat J, et al. (2025) The CH4/CO2 Gas Mixture Separation Using the Graphene, SiC, and BN Nanochannels: A Comprehensive Computational Approach. ACS omega, 10(30), 33295.

Paciotti R, et al. (2025) Unprecedented carbonic anhydrase inhibition mechanism: Targeting histidine 64 side chain through a halogen bond. Archiv der Pharmazie, 358(1), e2400776.

Muñiz-Chicharro A, et al. (2025) A Multiscale Simulation Approach to Compute Protein-Ligand Association Rate Constants by Combining Brownian Dynamics and Molecular Dynamics. Journal of chemical information and modeling, 65(20), 11215.

Kumar A, et al. (2025) Molecular dynamics simulation and docking studies reveals inhibition of NF-kB signaling as a promising therapeutic drug target for reduction in cytokines storms. Scientific reports, 15(1), 15225.

Singh BG, et al. (2025) Experimental and Theoretical Studies on Reaction Kinetics, Mechanism, and Degradation of Quinoline-Based Herbicide with Hydroxyl Radical, Sulphate Radical Anion, and Hydrated Electron. Chemphyschem : a European journal of chemical physics and physical chemistry, 26(13), e202401135.

Nem?ovi?ová I, et al. (2025) Small glycomimetic antagonists of the cytomegalovirus glycoprotein UL141 prevent binding to TRAIL death receptor. The Journal of biological chemistry, 301(5), 108490.

Randi PAS, et al. (2025) Stabilization Method as a Tool for Electronic State Spectroscopy. The journal of physical chemistry. A, 129(26), 5820.

Salvi E, et al. (2025) On the Role of Electronic Correlation and State-Specific Environment Polarization in Singlet-Triplet Gap Inversion. Journal of computational chemistry, 46(30), e70267.

Alrubia S, et al. (2025) Spectrophotometric and computational characterization of charge transfer complex of selumetinib with 2,3-dichloro-5,6-dicyano-1,4-benzoquinone and its utilization in developing an innovative green and high throughput microwell assay for analysis of bulk form and pharmaceutical formulation. BMC chemistry, 19(1), 27.

Ibragimov S, et al. (2025) Isomers of Iron(III) Oxides and Cobalt(III) Oxides and Their Redox Properties: Quantum-Chemical Insights. Molecules (Basel, Switzerland), 30(21).

Ghavi Z, et al. (2025) Molecular dynamics insights into non-covalent functionalization of boron nitride nanotubes for doxorubicin delivery. Scientific reports, 15(1), 30213.

Lai R, et al. (2025) Mechanism of Ampicillin Hydrolysis by New Delhi Metallo-?-Lactamase 1: Insight From QM/MM MP2 Calculation. Journal of computational chemistry, 46(1), e27544.

Pompon D, et al. (2025) Geometry-encoded molecular dynamics enables deep learning insights into P450 regiospecificity control. Scientific reports, 15(1), 7512.

Gade P, et al. (2025) Different chemical scaffolds bind to L-phe site in Mycobacterium tuberculosis Phe-tRNA synthetase. European journal of medicinal chemistry, 287, 117335.

Ali Q, et al. (2025) Assessment of the potential and application of Be12O12 nanocage for removal of ciprofloxacin from water employing density functional theory. Scientific reports, 15(1), 1020.

Serrano-Morrás Á, et al. (2025) The Quasi-Bound State as a Predictor of Relative Binding Free Energy. Journal of chemical information and modeling, 65(11), 5544.

Saito K, et al. (2025) Identification and design principles of far-red-absorbing chlorophyll in the light-harvesting complex. The Journal of biological chemistry, 301(6), 108518.

Zandi P, et al. (2025) Detecting Cr6+ at ?100 pM Concentration with Fluorescence Enhancement Signatures in a Novel Eco-Fluorophore: Matching WHO's 96 pM Recommended Standard for Drinking Water. Advanced materials (Deerfield Beach, Fla.), 37(29), e2504142.

Ruiz-Gonzalez A, et al. (2025) Calcium Ion Sensors with Unrivaled Stability and Selectivity Using a Bilayer Approach with Ionically Imprinted Nanocomposites. Nanomaterials (Basel, Switzerland), 15(10).

Tsuneda T, et al. (2025) Bridging electron and nuclear motions in chemical reactions through electrostatic forces from reactive orbitals. Communications chemistry, 8(1), 158.