Resource Summary Report

Generated by RRID on Sep 19, 2026

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: software resource, source code

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

Record Creation Time: 20220129T080322+0000

Record Last Update: 20260919T195916+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 279 mentions in open access literature.

Listed below are recent publications. The full list is available at RRID .

Ince C, et al. (2026) Effect of temperature on interactions between soy 11S glycinin and hexanal - An off-flavour compound. Food chemistry. Molecular sciences, 12, 100379.

Corallo AA, et al. (2026) Targeting TRPA1 with Novel Synthetic Compounds Based on Different Scaffolds to Reduce Acute and Chronic Pain. International journal of molecular sciences, 27(4).

Halenkovi?? T, et al. (2026) Cluster-based DFT modeling of Raman vibrations in tetrahedral GeS2 and GeSe2 amorphous chalcogenides. Scientific reports, 16(1).

Guerra P, et al. (2026) The Role of Benzonitrile Chlorination Explored by Dissociative Electron Attachment. Chemphyschem : a European journal of chemical physics and physical chemistry, 27(9), e70406.

Noji T, et al. (2026) Molecular basis for alternative charge separation pathways in type-II photosynthetic reaction centers. PNAS nexus, 5(4), pgag111.

Fukumoto Y, et al. (2026) Energetically equivalent structural transitions in the Rad17-Rad9-Hus1-Rad1-Rhino complex underlie the sequential progression from activation through maintenance to inactivation of the ATR-dependent DNA damage response. Nucleic acids research, 54(4).

Pyun WY, et al. (2026) Nutrient Availability Dictates Cancer Metabolism-Based Therapeutic Responses to Nononcology Drugs. Cancer research, 86(5), 1194.

Betkhoshvili S, et al. (2026) Aromaticity-Induced Spin State Switching and High-Spin States in Non-Alternant Polyradicals. Journal of computational chemistry, 47(10), e70366.

Fukumoto Y, et al. (2026) Reactive sulfur species are inactivated and excreted as trimethylsulfonium ion by thiopurine S-methyltransferase. Redox biology, 93, 104144.

Torkamanasadi M, et al. (2026) Surface-Bulk Correlation Spectroscopy for the Characterization of Ternary Adsorption. Applied spectroscopy, 80(6), 577.

Thalmann KS, et al. (2026) Unraveling Charge and Energy Transfer in a Singlet Fission Donor-Acceptor Complex: An Ab Initio Quantum Dynamical Study. Journal of chemical theory and computation, 22(5), 2129.

Viegas LP, et al. (2026) Modeling Radiative Efficiency across Fluorinated Molecules: Bridging Chemistry and Climate Policy for Global Warming Potential Estimations. Environmental science & technology, 60(8), 6188.

Jiang Y, et al. (2026) Photocatalytic C-C Coupling by a Au(I) Complex: Mechanistic Elucidation and SET Modulation. JACS Au, 6(2), 1148.

Ibrahim PEGF, et al. (2026) FMOPhore for hotspot identification and efficient fragment-to-lead growth strategies. Nature communications, 17(1).

Kwon S, et al. (2026) Ultrafast Cation-Dication Dynamics in Ammonia Borane: H-Migration to Roaming H2 and Reduced H3+ Formation under Strong-Field Ionization. The journal of physical chemistry. A, 130(9), 1780.

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.

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.

Love AM, et al. (2025) Reversal of the Leloir pathway to promote galactose and tagatose synthesis from glucose. Cell reports. Physical science, 6(12).

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.