AIP | The Journal of Chemical Physics

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Going forward, the Journal will continue to publish Communications, Perspectives, Special Topic sections, and regular articles in core areas of chemical physics as well as emerging and multidisciplinary fields. The Journal covers the latest breakthroughs in theoretical methods and advanced experimental techniques in chemical physics relevant to studies of atoms, molecules, clusters, liquids, glasses, crystals, polymers, biological molecules and networks, surfaces, interfaces, and materials.

Here are 80 articles that highlight the 80 years of outstanding work published in the Journal.
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Kinetics of Phase Change. I General Theory
Melvin Avrami
J. Chem. Phys. **7**, 1103 (1939)

Dispersion and Absorption in Dielectrics I. Alternating Current Characteristics
Kenneth S. Cole and Robert H. Cole
J. Chem. Phys. **9**, 341 (1941)

The Activated Complex in Chemical Reactions
Henry Eyring
J. Chem. Phys. **3**, 107 (1935)

A Theory of Water and Ionic Solution, with Particular Reference to Hydrogen and Hydroxyl Ions
J. D. Bernal and R. H. Fowler
J. Chem. Phys. **1**, 515 (1933)

Thermodynamics of High Polymer Solutions
Paul J. Flory
J. Chem. Phys. **10**, 51 (1942)

Solutions of Long Chain Compounds
Maurice L. Huggins
J. Chem. Phys. **9**, 440 (1941)

A New Electroaffinity Scale; Together with Data on Valence States and on Valence Ionization Potentials and Electron Affinities
Robert S. Mulliken
J. Chem. Phys. **2**, 782 (1934)

Statistical Mechanics of Fluid Mixtures
John G. Kirkwood
J. Chem. Phys. **3**, 300 (1935)

On the Isotopic Chemistry of Carbonates and a Paleotemperature Scale
J. M. McCrea
J. Chem. Phys. **18**, 849 (1950)

Free Volume and Entropy in Condensed Systems III. Entropy in Binary Liquid Mixtures; Partial Molal Entropy in Dilute Solutions; Structure and Thermodynamics in Aqueous Electrolytes
Henry S. Frank and Marjorie W. Evans
J. Chem. Phys. **13**, 507 (1945)

The Franck-Condon Principle and Its Application to Crystals
Melvin Lax
J. Chem. Phys. **20**, 1752 (1952)

The Spectra and Electronic Structure of the Tetrahedral Ions MnO_4^-, CrO_4^{--}, and ClO_4^-
Max Wolfsberg and Lindsay Helmholz
J. Chem. Phys. **20**, 837 (1952)

On the Non-Orthogonality Problem Connected with the Use of Atomic Wave Functions in the Theory of Molecules and Crystals
Per-Olov Löwdin
J. Chem. Phys. **18**, 365 (1950)

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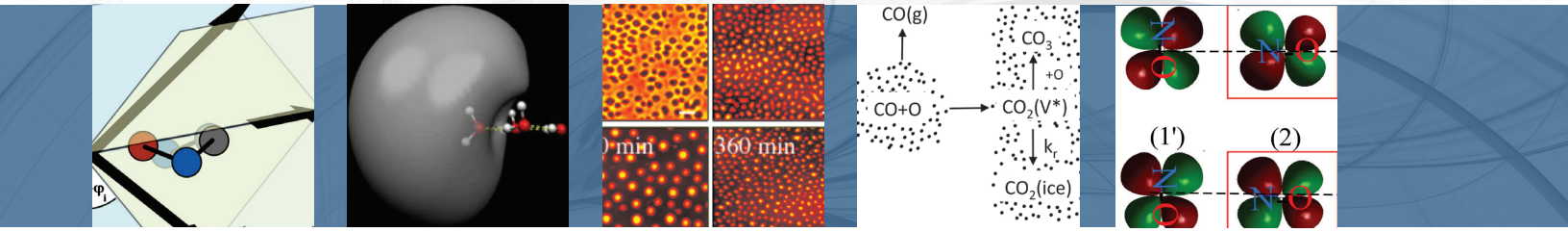

Determination of Electronic Structure of Molecules from Nuclear Quadrupole Effects
C. H. Townes and B. P. Dailey
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The Effect of Droplet Size on Surface Tension
Richard C. Tolman
J. Chem. Phys. **17**, 333 (1949)

Calculation of Vibrational Relaxation Times in Gases
R. N. Schwartz, Z. I. Slawsky, and K. F. Herzfeld
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Equation of State Calculations by Fast Computing Machines
Nicholas Metropolis, Arianna W. Rosenbluth, Marshall N. Rosenbluth, Augusta H. Teller, and Edward Teller
J. Chem. Phys. **21**, 1087 (1953)

A Theory of Sensitized Luminescence in Solids
D. L. Dexter
J. Chem. Phys. **21**, 836 (1953)

Intensities of Crystal Spectra of Rare-Earth Ions
G. S. Ofelt
J. Chem. Phys. **37**, 511 (1962)

On the Theory of Oxidation-Reduction Reactions Involving Electron Transfer. I
R. A. Marcus
J. Chem. Phys. **24**, 966 (1956)

A Theory of the Linear Viscoelastic Properties of Dilute Solutions of Coiling Polymers
Prince E. Rouse
J. Chem. Phys. **21**, 1272 (1953)

Contact Electron-Spin Coupling of Nuclear Magnetic Moments
Martin Karplus
J. Chem. Phys. **30**, 11 (1959)

Ensemble Method in the Theory of Irreversibility
Robert Zwanzig
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Relationship between Absorption Intensity and Fluorescence Lifetime of Molecules
S. J. Strickler and Robert A. Berg
J. Chem. Phys. **37**, 814 (1962)

Equation of State for Nonattracting Rigid Spheres
Norman F. Carnahan and Kenneth E. Starling
J. Chem. Phys. **51**, 635 (1969)

Spin Diffusion Measurements: Spin Echoes in the Presence of a Time-Dependent Field Gradient
E. O. Stejskal and J. E. Tanner
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Raman Spectrum of Graphite
F. Tuinstra and J. L. Koenig
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An Extended Hückel Theory. I. Hydrocarbons
Roald Hoffmann
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Relativistic Calculation of Anomalous Scattering Factors for X Rays
Don T. Cromer and David Liberman
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Coherent X-Ray Scattering for the Hydrogen Atom in the Hydrogen Molecule
Robert F. Stewart, Ernest R. Davidson, and William T. Simpson
J. Chem. Phys. **42**, 3175 (1965)

On the Temperature Dependence of Cooperative Relaxation Properties in Glass-Forming Liquids
Gerold Adam and Julian H. Gibbs
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Some Topics in the Theory of Fluids
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Contracted Gaussian basis sets for molecular calculations. I. Second row atoms, Z=11–18
A. D. McLean and G. S. Chandler
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A full coupled-cluster singles and doubles model: The inclusion of disconnected triples
George D. Purvis and Rodney J. Bartlett
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Investigation of exchange processes by two-dimensional NMR spectroscopy
J. Jeener, B. H. Meier, P. Bachmann, and R. R. Ernst
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John W. Cahn
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Self-consistent molecular orbital methods. XXIII. A polarization-type basis set for second-row elements
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Eric J. Heller
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Proton-enhanced NMR of dilute spins in solids
A. Pines, M. G. Gibby, and J. S. Waugh
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William C. Swope, Hans C. Andersen, Peter H. Berens, and Kent R. Wilson
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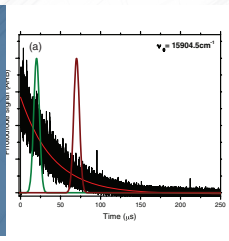

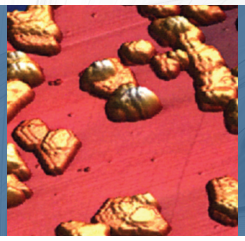
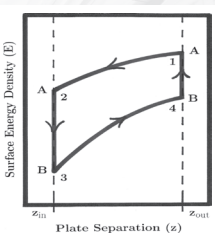

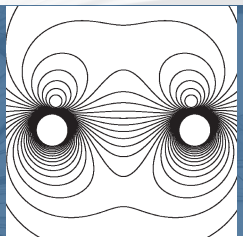
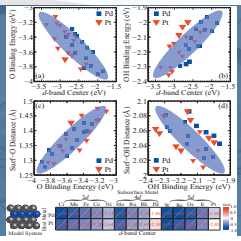

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Axel D. Becke
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Gaussian basis sets for use in correlated molecular calculations. I. The atoms boron through neon and hydrogen
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Comparison of simple potential functions for simulating liquid water
William L. Jorgensen, Jayaraman Chandrasekhar, Jeffry D. Madura, Roger W. Impey, and Michael L. Klein
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Toward reliable density functional methods without adjustable parameters: The PBE0 model
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J. Chem. Phys. **110**, 6158 (1999)

Molecular excitation energies to high-lying bound states from time-dependent density-functional response theory: Characterization and correction of the time-dependent local density approximation ionization threshold
Mark E. Casida, Christine Jamorski, Kim C. Casida, and Dennis R. Salahub
J. Chem. Phys. **108**, 4439 (1998)

An efficient implementation of time-dependent density-functional theory for the calculation of excitation energies of large molecules
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J. Chem. Phys. **109**, 8218 (1998)

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Tom Darden, Darrin York, and Lee Pedersen
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Graeme Henkelman, Blas P. Uberuaga, and Hannes Jónsson
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Improved second-order Møller–Plesset perturbation theory by separate scaling of parallel- and antiparallel-spin pair correlation energies
Stefan Grimme
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Hybrid coupled cluster and molecular dynamics approach: Application to the excitation spectrum of cytosine in the native DNA environment
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Solving the Schrödinger equation for helium atom and its isoelectronic ions with the free iterative complement interaction (ICI) method
Hiroyuki Nakashima and Hiroshi Nakatsuji
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Werner Kutzelnigg
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Time-resolved specular and off-specular neutron reflectivity measurements on deuterated polystyrene and poly(vinyl methyl ether) blend thin films during dewetting process
Hiroki Ogawa, Toshiji Kanaya, Koji Nishida, Go Matsuba, Jaroslaw P. Majewski, and Erik Watkins
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Growing correlation length in supercooled water
Emily B. Moore and Valeria Molinero
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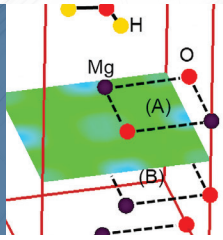

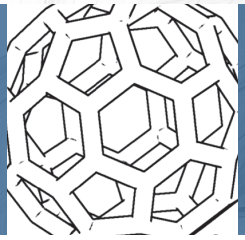
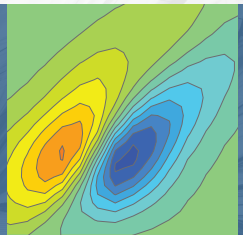
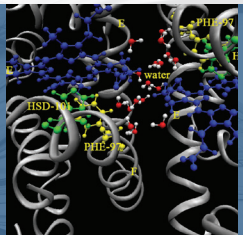
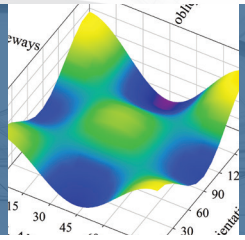

Photofragment angular momentum distributions in the molecular frame II. Single state dissociation, multiple state interference, and nonaxial recoil in photodissociation of polyatomic molecules
T. Peter Rakitzis and Andrew J. Alexander
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Communications: Exceptions to the d-band model of chemisorption on metal surfaces: The dominant role of repulsion between adsorbate states and metal d-states
Hongliang Xin and Suljo Linic
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Roderick C. I. MacKenzie, Jarvist M. Frost, and Jenny Nelson
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David W. Chandler and Kevin E. Strecker
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Stephen T. Edwards, Mark A. Johnson, and John C. Tully
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Systematic coarse-graining of potential energy landscapes and dynamics in liquids
M. Scott Shell
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Xiaojun Cai, Bian Hu, Ting Sun, Kevin F. Kelly, and Steven Baldelli
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S. Capaccioli and K. L. Ngai
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Communication maps computed for homodimeric hemoglobin: Computational study of water-mediated energy transport in proteins
Ramachandran Gnanasekaran, Johnson K. Agbo, and David M. Leitner
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Stereo correlated dynamics in the energy transfer process of aligned N_2 ($A\ ^3\Sigma_u^+$) + oriented NO ($X\ ^2\Pi$, $\Omega = 1/2$) $\rightarrow$ NO ($A\ ^2\Sigma^+$) + N_2 ($X\ ^1\Sigma_g^+$)
H. Ohoyama and S. Maruyama
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Chunqing Yuan and John T. Yates, Jr.
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Lorenz S. Cederbaum
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Enhancement of molecular modes by electronically resonant multipulse excitation: Further progress towards mode selective chemistry
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