



*The Journal of Chemical Physics* is proud to be celebrating its 80th year as the leading and most cited journal in chemical physics. The Journal has been at the forefront of the field since its inception in 1933. The 80th Anniversary Collection includes seminal papers on electronic structure methods, potential energy surfaces, transition states and reaction pathways, Monte Carlo and molecular dynamics simulation methods and applications, time-dependent methods in quantum dynamics, electron transfer reactions, advances in nuclear magnetic resonance methods, and spectroscopic methods and formalisms including multidimensional techniques with applications ranging from water to proteins.

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. Happy 80th Anniversary to *The Journal of Chemical Physics!*

#### **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**

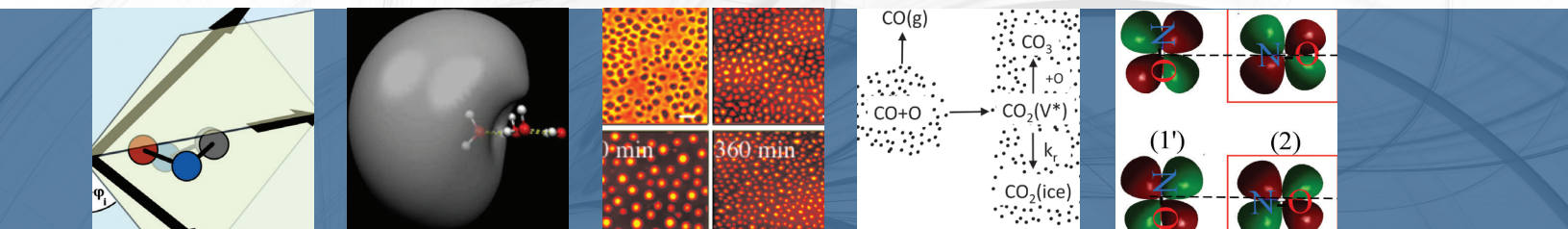
Melvin Lax  
J. Chem. Phys. **20**, 1752 (1952)

#### **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)



### Determination of Electronic Structure of Molecules from Nuclear Quadrupole Effects

C. H. Townes and B. P. Dailey  
*J. Chem. Phys.* **17**, 782 (1949)

### 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  
*J. Chem. Phys.* **20**, 1591 (1952)

### 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  
*J. Chem. Phys.* **33**, 1338 (1960)

### 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  
*J. Chem. Phys.* **42**, 288 (1965)

### Raman Spectrum of Graphite

F. Tuinstra and J. L. Koenig  
*J. Chem. Phys.* **53**, 1126 (1970)

### An Extended Hückel Theory. I. Hydrocarbons

Roald Hoffmann  
*J. Chem. Phys.* **39**, 1397 (1963)

### Relativistic Calculation of Anomalous Scattering Factors for X Rays

Don T. Cromer and David Liberman  
*J. Chem. Phys.* **53**, 1891 (1970)

### 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  
*J. Chem. Phys.* **43**, 139 (1965)

### Some Topics in the Theory of Fluids

B. Widom  
*J. Chem. Phys.* **39**, 2808 (1963)

### Contracted Gaussian basis sets for molecular calculations. I. Second row atoms, Z=11-18

A. D. McLean and G. S. Chandler  
*J. Chem. Phys.* **72**, 5639 (1980)

### A full coupled-cluster singles and doubles model: The inclusion of disconnected triples

George D. Purvis and Rodney J. Bartlett  
*J. Chem. Phys.* **76**, 1910 (1982)

### Investigation of exchange processes by two-dimensional NMR spectroscopy

J. Jeener, B. H. Meier, P. Bachmann, and R. R. Ernst  
*J. Chem. Phys.* **71**, 4546 (1979)

### Critical point wetting

John W. Cahn  
*J. Chem. Phys.* **66**, 3667 (1977)

### Self-consistent molecular orbital methods. XXIII. A polarization-type basis set for second-row elements

Michelle M. Francl, William J. Pietro, Warren J. Hehre, J. Stephen Binkley, Mark S. Gordon, Douglas J. DeFrees, and John A. Pople  
*J. Chem. Phys.* **77**, 3654 (1982)

### Time-dependent approach to semiclassical dynamics

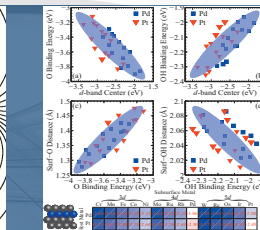
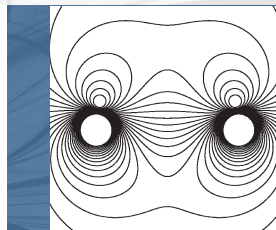
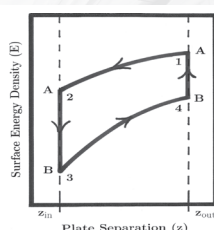
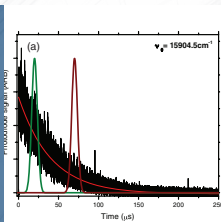
Eric J. Heller  
*J. Chem. Phys.* **62**, 1544 (1975)

### Proton-enhanced NMR of dilute spins in solids

A. Pines, M. G. Gibby, and J. S. Waugh  
*J. Chem. Phys.* **59**, 569 (1973)

### A computer simulation method for the calculation of equilibrium constants for the formation of physical clusters of molecules: Application to small water clusters

William C. Swope, Hans C. Andersen, Peter H. Berens, and Kent R. Wilson  
*J. Chem. Phys.* **76**, 637 (1982)



### Density-functional thermochemistry. III. The role of exact exchange

Axel D. Becke  
J. Chem. Phys. **98**, 5648 (1993)

### Gaussian basis sets for use in correlated molecular calculations. I. The atoms boron through neon and hydrogen

Thom H. Dunning  
J. Chem. Phys. **90**, 1007 (1989)

### Comparison of simple potential functions for simulating liquid water

William L. Jorgensen, Jayaraman Chandrasekhar, Jeffry D. Madura, Roger W. Impey, and Michael L. Klein  
J. Chem. Phys. **79**, 926 (1983)

### Ab initio effective core potentials for molecular calculations. Potentials for K to Au including the outermost core orbitals

P. Jeffrey Hay and Willard R. Wadt  
J. Chem. Phys. **82**, 299 (1985)

### A unified formulation of the constant temperature molecular dynamics methods

Shuichi Nosé  
J. Chem. Phys. **81**, 511 (1984)

### An all-electron numerical method for solving the local density functional for polyatomic molecules

B. Delley  
J. Chem. Phys. **92**, 508 (1990)

### An improved algorithm for reaction path following

Carlos Gonzalez and H. Bernhard Schlegel  
J. Chem. Phys. **90**, 2154 (1989)

### Second-order perturbation theory with a complete active space self-consistent field reference function

Kerstin Andersson, Per-Åke Malmqvist, and Björn O. Roos  
J. Chem. Phys. **96**, 1218 (1992)

### Toward reliable density functional methods without adjustable parameters: The PBE0 model

Carlo Adamo and Vincenzo Barone  
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

R. Eric Stratmann, Gustavo E. Scuseria, and Michael J. Frisch  
J. Chem. Phys. **109**, 8218 (1998)

### Particle mesh Ewald: $N\log(N)$ method for Ewald sums in large systems

Tom Darden, Darrin York, and Lee Pedersen  
J. Chem. Phys. **98**, 10089 (1993)

### A climbing image nudged elastic band method for finding saddle points and minimum energy paths

Graeme Henkelman, Blas P. Uberuaga, and Hannes Jónsson  
J. Chem. Phys. **113**, 9901 (2000)

### A new integral equation formalism for the polarizable continuum model: Theoretical background and applications to isotropic and anisotropic dielectrics

E. Cancès, B. Mennucci, and J. Tomasi  
J. Chem. Phys. **107**, 3032 (1997)

### Improved second-order Møller-Plesset perturbation theory by separate scaling of parallel- and antiparallel-spin pair correlation energies

Stefan Grimme  
J. Chem. Phys. **118**, 9095 (2003)

### Hybrid coupled cluster and molecular dynamics approach: Application to the excitation spectrum of cytosine in the native DNA environment

Marat Valiev and Karol Kowalski  
J. Chem. Phys. **125**, 211101 (2006)

### Solving the Schrödinger equation for helium atom and its isoelectronic ions with the free iterative complement interaction (ICI) method

Hiroyuki Nakashima and Hiroshi Nakatsuji  
J. Chem. Phys. **127**, 224104 (2007)

### Density-cumulant functional theory

Werner Kutzelnigg  
J. Chem. Phys. **125**, 171101 (2006)

### Free energies of stable and metastable pores in lipid membranes under tension

Wouter K. den Otter  
J. Chem. Phys. **131**, 205101 (2009)

### 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  
J. Chem. Phys. **131**, 104907 (2009)

### Casimir chemistry

D. P. Sheehan  
J. Chem. Phys. **131**, 104706 (2009)

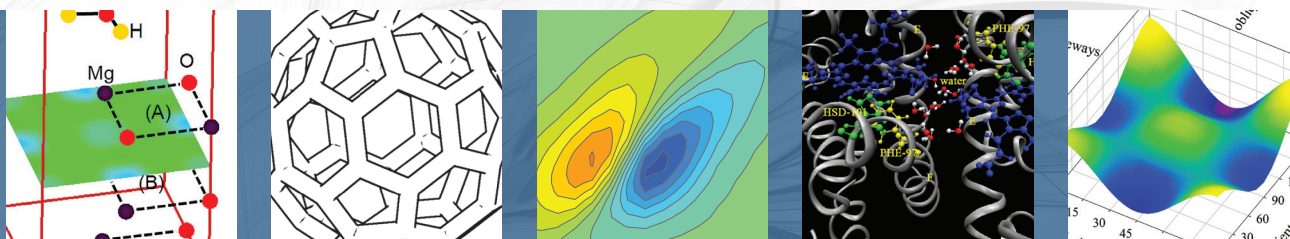
### Growing correlation length in supercooled water

Emily B. Moore and Valeria Molinero  
J. Chem. Phys. **130**, 244505 (2009)

### Rung 3.5 density functionals

Benjamin G. Janesko  
J. Chem. Phys. **133**, 104103 (2010)





**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  
*J. Chem. Phys.* **132**, 224310 (2010)

**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  
*J. Chem. Phys.* **132**, 221101 (2010)

**A numerical study of mobility in thin films of fullerene derivatives**

Roderick C. I. MacKenzie, Jarvist M. Frost, and Jenny Nelson  
*J. Chem. Phys.* **132**, 064904 (2010)

**Dual-etalon frequency-comb cavity ringdown spectrometer**

David W. Chandler and Kevin E. Strecker  
*J. Chem. Phys.* **136**, 154201 (2012)

**Vibrational Fano resonances in dipole-bound anions**

Stephen T. Edwards, Mark A. Johnson, and John C. Tully  
*J. Chem. Phys.* **136**, 154305 (2012)

**Systematic coarse-graining of potential energy landscapes and dynamics in liquids**

M. Scott Shell  
*J. Chem. Phys.* **137**, 084503 (2012)

**Potential-functional embedding theory for molecules and materials**

Chen Huang and Emily A. Carter  
*J. Chem. Phys.* **135**, 194104 (2011)

**Sum frequency generation-compressive sensing microscope**

Xiaojun Cai, Bian Hu, Ting Sun, Kevin F. Kelly, and Steven Baldelli  
*J. Chem. Phys.* **135**, 194202 (2011)

**Resolving the controversy on the glass transition temperature of water?**

S. Capaccioli and K. L. Ngai  
*J. Chem. Phys.* **135**, 104504 (2011)

**Communication maps computed for homodimeric hemoglobin: Computational study of water-mediated energy transport in proteins**

Ramachandran Gnanasekaran, Johnson K. Agbo, and David M. Leitner  
*J. Chem. Phys.* **135**, 065103 (2011)

**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  
*J. Chem. Phys.* **137**, 064311 (2012)

**Isotope effect in the photochemical decomposition of  $CO_2$  (ice) by Lyman- $\alpha$  radiation**

Chunqing Yuan and John T. Yates, Jr.  
*J. Chem. Phys.* **138**, 154302 (2013)

**Quantification of transition dipole strengths using 1D and 2D spectroscopy for the identification of molecular structures via exciton delocalization: Application to  $\alpha$ -helices**

Maksim Grechko and Martin T. Zanni  
*J. Chem. Phys.* **137**, 184202 (2012)

**The exact molecular wavefunction as a product of an electronic and a nuclear wavefunction**

Lorenz S. Cederbaum  
*J. Chem. Phys.* **138**, 224110 (2013)

**Enhancement of molecular modes by electronically resonant multipulse excitation: Further progress towards mode selective chemistry**

Jürgen Hauer, Tiago Buckup, and Marcus Motzkus  
*J. Chem. Phys.* **125**, 061101 (2006)

**A simple model of molecular electronic devices and its analytical solution**

Matthias Ernzerhof  
*J. Chem. Phys.* **127**, 204709 (2007)

**A molecular view of heterogeneous catalysis**

Claus Hviid Christensen and Jens K. Nørskov  
*J. Chem. Phys.* **128**, 182503 (2008)