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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. 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

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

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

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$_4^{2-}$, 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
J. Chem. Phys. 17, 782 (1949)

The Effect of Droplet Size on Surface Tension
Richard C. Tolman

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
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

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

Ensemble Method in the Theory of Irreversibility
Robert Zwanzig

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

Spin Diffusion Measurements: Spin Echoes in the Presence of a Time-Dependent Field Gradient
E. O. Stejskal and J. E. Tanner

Raman Spectrum of Graphite
F. Tuinstra and J. L. Koenig

An Extended Hückel Theory. I. Hydrocarbons
Roald Hoffmann

Relativistic Calculation of Anomalous Scattering Factors for X Rays
Don T. Cromer and David Liberman

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
Gerald Adam and Julian H. Gibbs
J. Chem. Phys. 43, 139 (1965)

Some Topics in the Theory of Fluids
B. Widom

Contracted Gaussian basis sets for molecular calculations. I. Second row atoms, Z=11–18
A. D. McLean and G. S. Chandler

A full coupled-cluster singles and doubles model: The inclusion of disconnected triples
George D. Purvis and Rodney J. Bartlett

Investigation of exchange processes by two-dimensional NMR spectroscopy
J. Jeener, B. H. Meier, P. Bachmann, and R. R. Ernst

Critical point wetting
John W. Cahn

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

Time-dependent approach to semiclassical dynamics
Eric J. Heller

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
Density-functional thermochemistry. III. The role of exact exchange
Axel D. Becke

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

Comparison of simple potential functions for simulating liquid water
William L. Jorgensen, Jayaraman Chandrasekhar, Jeffry D. Madura, Roger W. Impey, and Michael L. Klein

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

An all-electron numerical method for solving the local density functional for polyatomic molecules
B. Delley

An improved algorithm for reaction path following
Carlos Gonzalez and H. Bernhard Schlegel

Second-order perturbation theory with a complete active space self-consistent field reference function
Kerstin Andersson, Per-Åke Malmqvist, and Bjorn O. Roos

Toward reliable density functional methods without adjustable parameters: The PBE0 model
Carlo Adamo and Vincenzo Barone

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

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

Particle mesh Ewald: N-log(N) method for Ewald sums in large systems
Tom Darden, Darrin York, and Lee Pedersen

A climbing image nudged elastic band method for finding saddle points and minimum energy paths
Graeme Henkelman, Blas P. Uberuaga, and Hannes Jónsson

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

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

Hybrid coupled cluster and molecular dynamics approach: Application to the excitation spectrum of cytosine in the native DNA environment
Marat Valiev and Karol Kowalski

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

Density-cumulant functional theory
Werner Kutzelnigg

Free energies of stable and metastable pores in lipid membranes under tension
Wouter K. den Otter

Time-resolved specular and off-specular neutron reflectivity measurements on deuterated polystyrene and poly(vinyl methyl ether) blend thin films during dewetting process
Hiromi Oikawa, Toshiji Kanaya, Koji Nishida, Go Matsuba, Jaroslaw P. Majewski, and Erik Watkins

Casimir chemistry
D. P. Sheehan

Growing correlation length in supercooled water
Emily B. Moore and Valeria Molinero

Rung 3.5 density functionals
Benjamin G. Janesko
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

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

A numerical study of mobility in thin films of fullerene derivatives
Roderick C. I. MacKenzie, Jarvist M. Frost, and Jenny Nelson

Dual-etalon frequency-comb cavity ringdown spectrometer
David W. Chandler and Kevin E. Strecker

Vibrational Fano resonances in dipole-bound anions
Stephen T. Edwards, Mark A. Johnson, and John C. Tully

Systematic coarse-graining of potential energy landscapes and dynamics in liquids
M. Scott Shell

Potential-functional embedding theory for molecules and materials
Chen Huang and Emily A. Carter

Sum frequency generation-compressive sensing microscope
Xiaojun Cai, Bian Hu, Ting Sun, Kevin F. Kelly, and Steven Baldelli

Resolving the controversy on the glass transition temperature of water?
S. Capaccioli and K. L. Ngai

Communication maps computed for homodimeric hemoglobin: Computational study of water-mediated energy transport in proteins
Ramachandran Gnanasekaran, Johnson K. Abo, and David M. Leitner

Stereo correlated dynamics in the energy transfer process of aligned N₂ (A ³Σ⁺) + oriented NO (X ²Π, Ω = 1/2) → NO (A ²Σ⁺) + N₂ (X ¹Σ⁺)
H. Ohoyama and S. Maruyama

Isotope effect in the photochemical decomposition of CO₂ (ice) by Lyman-α radiation
Chunqing Yuan and John T. Yates, Jr.

Quantification of transition dipole strengths using 1D and 2D spectroscopy for the identification of molecular structures via exciton delocalization: Application to α-helices
Maksim Grechko and Martin T. Zanni

The exact molecular wavefunction as a product of an electronic and a nuclear wavefunction
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Enhancement of molecular modes by electronically resonant multipulse excitation: Further progress towards mode selective chemistry
Jurgen Hauer, Tiago Buckup, and Marcus Motzkus

A simple model of molecular electronic devices and its analytical solution
Matthias Ernzerhof

A molecular view of heterogeneous catalysis
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