

THE JOURNAL OF CHEMICAL PHYSICS

CODEN: JCPSA6

ISSN: 0021-9606

<http://ojps.aip.org/jcpo>

Editor: Donald Levy

Senior Associate Editor: John Light,
The University of Chicago, Chicago, IL

Associate Editors:

Marshall Fixman, Branka Ladanyi,
Colorado State University, Fort Collins, CO

Ernest Davidson, *University of Washington, Seattle, WA*

Horia Metiu, *University of California, Santa Barbara, CA*

Editorial Board

Term ending 31 December 2003

David M. Bishop (University of Ottawa, Ottawa, Ontario, Canada)

R. B. Gerber (Hebrew University, Jerusalem, Israel)

Kenneth D. Jordan (University of Pittsburgh, Pittsburgh, PA)

Kevin K. Lehmann (Princeton University, Princeton, NJ)

Robert J. LeRoy (University of Waterloo, Waterloo, Ontario, Canada)

Mark Maroncelli (Pennsylvania State University, University Park, PA)

Hanna Reisler (University of Southern California, Los Angeles, CA)

Alec M. Wodtke (University of California, Santa Barbara, CA)

Term ending 31 December 2004

Moungi G. Bawendi (MIT, Cambridge, MA)

Charles T. Campbell (University of Washington, Seattle, WA)

David C. Clary (University College London, London, UK)

Manfred M. Kappes (Universität Karlsruhe, Karlsruhe, Germany)

Jane E. G. Lipson (Dartmouth College, Hanover, NH)

David J. Nesbitt (JILA, University of Colorado, Boulder, CO)

Richard M. Stratt (Brown University, Providence, RI)

Robert Tycko (National Institutes of Health, Bethesda, MD)

Term ending 31 December 2005

Carol K. Hall (North Carolina State University, Raleigh, NC)

Wilson Ho (University of California, Irvine, CA)

James T. Hynes (Ecole Normale Supérieure, Paris, France)

William M. Jackson (University of California, Davis, CA)

Michael L. Klein (University of Pennsylvania, Philadelphia, PA)

James E. Martin (Sandia National Laboratories, Albuquerque, NM)

Gustavo E. Scuseria (Rice University, Houston, TX)

Arthur F. Voter (Los Alamos National Laboratory, Los Alamos, NM)

Information for Authors

Submissions: Submit manuscripts, as electronic PDF files, via the web-site: <http://jcp.uchicago.edu>. Do not send manuscripts to the editorial offices as e-mail attachments. If preferred, mail printed manuscripts (2 copies) to Donald Levy, Editor, *The Journal of Chemical Physics*, Department of Chemistry, 5735 S. Ellis Ave., The University of Chicago, Chicago, IL 60637; E-mail: editor@jcp.uchicago.edu; Fax: 773-702-8314. Submission implies that the manuscript has not been published previously and is not currently submitted for publication elsewhere. For detailed information for contributors, visit <http://ojps.aip.org/jcpo/jcpsubmit.jsp>.

Publication Charge: To support the cost of wide dissemination of research results through publication of journal pages and production of a database of articles, the author's institution is requested to pay a page charge of \$55 per page (with a one-page minimum) and an *article charge* of \$20 per article. For Errata the minimum page charge is \$10, with no article charge. For any regular article that exceeds 12 journal pages, the requested page charge is \$150 for each page in excess of 12 pages.

Color Printing: Color illustrations will be published free of charge to authors if the Journal's editors deem the use of color to be essential. For all other color figures, fixed rates of \$650 for the first color figure and \$325 for each additional color figure apply. For multipart figures, a single charge will apply only if all parts are submitted as a single piece of artwork.

Reprints: Order reprints with or without covers only in multiples of 50 from AIP, Circulation & Fulfillment/Reprints, Suite 1N01, 2 Huntington Quadrangle, Melville, NY 11747-4502; Fax: 516-349-9704; Tel.: 1-800-344-6909 (U.S. and Canada), or 516-576-2270.

Supplemental Material may be deposited with AIP's Electronic Physics Auxiliary Publication Service (EPAPS), a low-cost online depository. For a nominal fee, authors may submit multimedia, color figures, data tables, text, etc. Address requests to the Editor; for additional information, see <http://www.aip.org/pubserv/epaps.html>.

Online Status Inquiry: During the production process, authors may access information about their accepted manuscripts at <http://www.aip.org/msinq/status.html>.

Digital Object Identifier (DOI): Each archival article published is assigned a unique DOI that serves to identify the article in a digital environment. In print, the DOI appears at the end of each abstract.

The purpose of *The Journal of Chemical Physics* (JCP) is to bridge a gap between journals of physics and journals of chemistry by publishing quantitative research based on physical principles and techniques, as applied to "chemical" systems. Just as the fields of chemistry and physics have expanded, so have chemical physics subject areas which include polymers, materials, surfaces/interfaces, and biological macromolecules along with the traditional small molecule and condensed phase systems. JCP is published four times per month (48 issues per year) by the American Institute of Physics (AIP).

Comments: Direct comments on the journal or editorial process to Doreene Berger, Editorial Operations, AIP, Suite 1N01, 2 Huntington Quadrangle, Melville, NY 11747-4502. Tel.: 516-576-2444; Fax: 516-576-2450; E-mail: dberger@aip.org.

AIP Production Staff (E-mail: jcp@aip.org; Fax: 516-576-2643)

Doug Parker, *Team Manager*; Thomas Thrash, *Team Coordinator*; Carolyn De Marco, *Chief Production Editor*; Celeste Lentoni, *Senior Production Editor*; Joanne Barker, Jamie Frevele, Joanne Santangelo, *Production Editors*

2003 Subscription Prices

	USA & Poss.	Americas	RoW Surface	RoW Air
Print & online				
Members	\$379	\$564	\$564	\$694
Institutions	\$5,270	\$5,455		\$5,585

For Institutional subscriptions in Japan, contact AIP.

Microfiche & online (Rates apply for all subscriptions throughout the World.)

Members	\$379			
Institutions	\$5,270			

For Institutional subscriptions in Japan, contact AIP.

Print & quarterly CD & online

Members	\$444	\$629	\$629	\$759
Institutions	\$5,660	\$5,845		\$5,975

For Institutional subscriptions in Japan, contact AIP.

Quarterly CD & online

Members	\$322			
Institutions	\$4,480			

For Institutional subscriptions in Japan, contact AIP.

Online only (Rates apply for all subscriptions throughout the World.)

Members	\$170			
Institutions	\$3,955			

For Institutional subscriptions in Japan, contact AIP.

Online access covers 1998–2003; for access to backfiles from 1975 to present, add \$35 for Members and \$65 for Institutions.

Annual CD-ROM Add to subscription price: Members: \$30 Institutions: \$50

Single issues

Back issues for 2003: \$120 Prior years (Members): \$36 Prior years (Institutions): \$120 Before 1995: \$240

Additional Availability

Online Access: *The Journal of Chemical Physics* is available online at <http://ojps.aip.org/jcpo>.

Microform: *The Journal of Chemical Physics* is available on microfiche issued at the same frequency as the printed journal, and annually on microfilm. Direct requests to AIP, Circulation & Fulfillment/Single Copy Sales, Suite 1N01, 2 Huntington Quadrangle, Melville, NY 11747-4502; Fax: 516-349-9704; Tel.: 1-800-344-6902 (U.S. and Canada) or 516-576-2270.

Document Delivery: Copies of journal articles can be ordered for online delivery from DocumentStore, AIP's online document delivery service (<http://www.documentstore.org>).

Customer Service

Subscription Orders and Renewals should be addressed to American Institute of Physics, P.O. Box 503284, St. Louis, MO 63150-3284. Tel.: 1-800-344-6902 (U.S. and Canada) or 516-576-2270; Fax: 516-349-9704; E-mail: subs@aip.org. Allow at least six weeks advance notice.

Inquiries, Address Changes, Claims, Single Copy Replacements, and Back Volumes: For address changes, please send both old and new addresses and, if possible, include the mailing label from a recent issue. Missing issue requests will be honored only if received within six months of publication date (nine months for Australia and Asia). Single copies of a journal may be ordered and back volumes are available in print, microfiche, or microform. Contact AIP Customer Services at 1-800-344-6902 (U.S. and Canada) or 516-576-2270; Fax: 516-349-9704; E-mail: subs@aip.org.

Reprint Billing: Contact AIP Publication Charge and Reprints/CFD, Suite 1N01, 2 Huntington Quadrangle, Melville, NY 11747-4502; Tel.: 1-800-344-6909 (U.S. and Canada) or 516-576-2270; E-mail: pcr@aip.org.

Rights and Permissions

Copying: Single copies of individual articles may be made for private use or research. Authorization is given (as indicated by the Item Fee Code for this publication) to copy articles beyond the use permitted by Sections 107 and 108 of the U.S. Copyright Law, provided the copying fee of \$20 per copy per article is paid to the Copyright Clearance Center, 222 Rosewood Drive, Danvers, MA 01923, USA. Persons desiring to photocopy materials for classroom use should contact the CCC Academic Permissions Service. The Item Fee Code for this publication is 0021-9606/2003 \$20.00. Authorization does not extend to systematic or multiple reproduction, to copying for promotional purposes, to electronic storage or distribution, or to republication in any form. In all such cases, specific written permission from AIP must be obtained.

Other Use: Permission is granted to quote from the journal with the customary acknowledgment of the source. To reprint a figure, table, or other excerpt requires consent of one of the authors and notification to AIP. See journal home page for author's Web posting guidelines.

Requests for Permission: Address requests to AIP Office of Rights and Permissions, Suite 1N01, 2 Huntington Quadrangle, Melville, NY 11747-4502; Fax: 516-576-2450; Tel.: 516-576-2268; E-mail: rights@aip.org.

The Journal of Chemical Physics (ISSN: 0021-9606) is published four times per month, 48 issues per year by the American Institute of Physics. 2003 Subscription rates: US\$5270. POSTMASTER: Send address changes to *The Journal of Chemical Physics*, AIP, Suite 1N01, 2 Huntington Quadrangle, Melville, NY 11747-4502. Periodicals postage paid at Huntington Station, NY 11746, and additional mailing offices.

Copyright © 2003 American Institute of Physics. All rights reserved.