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A DETAILED MONTE CARLO INVESTIGATION OF THE TRICRITICAL REGION OF A BIAXIAL LIQUID CRYSTAL SYSTEM

CESARE CHICCOLI*, PAOLO PASINI†, and FRANCO SEMERIA‡

Instituto Nazionale di Fisica Nucleare, Sezione di Bologna, Via Irnerio 46, 40126 Bologna, Italy
**E-mail: chiccoli@bo.infn.it*
†*E-mail: pasini@bo.infn.it*
‡*E-mail: semeria@bo.infn.it*

CLAUDIO ZANNONI

Dipartimento di Chimica Fisica ed Inorganica dell' Università, Viale Risorgimento 4, 40136 Bologna, Italy
E-mail: vz3bod7a@sirio.cineca.it

We study a lattice system of biaxial particles interacting with a second-rank anisotropic potential. We have performed detailed Monte Carlo calculations in the vicinity of the prolate-oblate dual value of molecular biaxiality. Our results confirm the second-order character of the transition in this limiting case.

Keywords: Computer Simulations; Liquid Crystals; Biaxial Nematics.

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GUEST EDITORS' PREFACE

CESARE CHICCOLI and PAOLO PASINI

INFN Sezione di Bologna, Via Irnerio 46, 40126 Bologna, Italy

CLAUDIO ZANNONI

Dipartimento di Chimica Fisica ed Inorganica, Università di Bologna, Viale Risorgimento 4, 40136 Bologna, Italy

Recent Developments in the Computer Simulations of Liquid Crystals

Liquid crystals comprise a large number of fascinating states of soft condensed matter where the orientational order of the constituent molecules is associated with a reduced or absent translational order. This confers on liquid crystalline systems a combination of fluidity and easy alignment in external fields as well as anisotropic properties, similar to those of a crystal, that are the basis of their many technological applications in displays or other electro-optical devices. It is becoming increasingly clear that an understanding of the macroscopic properties of liquid crystals and of their phase transitions in terms of molecular models can only be attained using computer simulations, possibly with the complement of approximate statistical mechanical theories. Computer simulations are particularly interesting and timely now because of their very rapid development and wide reach. While simulations of liquid crystals are of course based on the same general Monte Carlo and Molecular Dynamics techniques used for other fluids, they present a number of problems and peculiarities connected with the intrinsic properties of liquid crystals, such as their long-range order and their anisotropy, that recommend a separate treatment. This in turn requires the development of suitable algorithms to calculate anisotropic static properties such as order parameters, correlation functions, elastic constants and, in general, tensorial observables as well as dynamic quantities such as diffusion tensors, viscosities, susceptivities etc. It is now also becoming possible to examine topological defects characteristic of the various liquid crystals and to investigate their core structure and even to perform direct microscopic-level simulations of simple devices and displays. Another series of problems is connected with the need for predicting the properties of liquid crystals from molecular models. This involves the determination of phase behavior, phase transitions and their characteristics, and requires the development of intermolecular potentials for modeling the essential molecular features of mesogens, as well as performing large-scale simulations with a number of particles, often an order of magnitude greater than those used in simple fluid simulations. This in itself requires exploiting state-of-the-art resources in computing, and particularly parallel computing techniques with the development of appropriate algorithms.

The meeting *Recent Developments in the Computer Simulations of Liquid Crystals* was held in Erice (Italy) on 18 June 1998 in association with a NATO ASI which covered all the above issues including the various techniques, model systems (from lattice to hard particle and Gay-Berne up to atomistic) for thermotropics, lyotropics and some liquid crystals of biological interest.

Some of the original contributions discussed at the meeting in Erice were submitted for these Proceedings and the papers that appear here were refereed according to the standard procedure of this Journal. As it can be seen from the papers of this issue, many computational aspects of liquid crystals were touched upon and we think that at least some of these are of general interest.

The success of the meeting was only possible thanks to the help of many people. We would like to mention particularly our collaborators R. Berardi, A. Porreca and S. Orlandi and the staff of CCSEM. Last but not least, the conference and the participation of many young researchers and students were only possible because of the essential support of the sponsors listed below that we warmly acknowledge.

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MONTE CARLO SIMULATIONS OF ROD-LIKE GAY-BERNE MESOGENS WITH TRANSVERSE DIPOLES

ROBERTO BERARDI, SILVIA ORLANDI, and CLAUDIO ZANNONI*

Departimento di Chimica Fisica ed Inorganica dell' Università, Viale Risorgimento 4, 40136 Bologna, Italy

**E-mail: vz3bod7a@sirio.cineca.it*

We report the results of a Monte Carlo investigation of a system of rod-like particles interacting via the Gay-Berne potential with an embedded transverse dipole. We describe the effect that the dipole has on the molecular organization.

Keywords: Computer Simulations; Liquid Crystals; Dipolar Systems.

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VIRIAL COEFFICIENTS FOR THE HARD GAUSSIAN OVERLAP MODEL

SSU-LI HUANG and VENKAT R. BHETHANABOTLA*

Department of Chemical Engineering, University of South Florida, Tampa, Florida 33620-5350
**E-mail: bhethana@eng.usf.edu*

Monte Carlo estimates of virial coefficients up to the sixth for the Hard Gaussian Overlap (HGO) model are presented for values of the aspect ratio parameter κ of the model ranging from 0.05 to 10. The sixth coefficients are new and the lower coefficients are improvements on previous numerical estimates. The second virials are found to be in excellent agreement with an analytical integration reported in the literature. Padé (3, 3) approximations to the pressure and residual Helmholtz energy were constructed. Attempts to represent coefficients in these approximations by analytical functions of κ were not successful due to singularities in these functions. In the approximate range of 4.5€≤€κ€≤€5.5, the (3, 3) Padé approximations were found to be no better than lower ones. Comparisons with available Monte Carlo simulated pressures for moderately aspherical fluids were found to be good.

Keywords: Virial Coefficients; Monte Carlo Integration; Nonspherical Molecules; Hard Body Models; Padé Approximation.

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LATERAL DIFFUSION OF FLEXIBLE LIPID CHAINS: A DYNAMIC MONTE CARLO STUDY

T. SINTES*, A. BAUMGÄRTNER, and Y. K. LEVINE†,‡

Forum Modelierung, Forschungszentrum, 52425 Jülich, Germany
**Present address: Instituto Mediterrano de Estudios Avanzados, IMEDEA (CSIC UIB), E-07071 Palma de Mallorca, Spain*
†*Permanant address: Debye Institute, Buys Ballot Laboratory, P.O. Box 80.000, 3508 TA Utrecht, The Netherlands*
‡*E-mail: Y.K.Levine@phys.uu.nl*

A computer simulation study of the lateral diffusion of conformationally-disordered lipid molecules in a monolayer structure is reported. The simulations were carried out with dynamic Monte Carlo methods, employing two different representations of the internal motions of the lipid chains. The results indicate that the dependence of the lateral diffusion coefficients on the density (area-per-molecule) in the monolayer is determined by the conformational behavior of the lipid chains. The classical Cohen-Turnbull theory is found to provide a good description of the simulated lateral diffusion coefficients at moderate densities. The substantial deviations found at low densities are attributed to the small density fluctuations creating the free volume needed for the lateral diffusion process.

Keywords: Lipid Chains; Lateral Diffusion; Computer Simulations; Lipid Monolayers; Dynamic Monte Carlo.

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ORIENTATION CORRELATION IN SIMPLIFIED MODELS OF POLYMER MELTS

ROLAND FALLER*, MATHIAS PÜTZ, and FLORIAN MÜLLER-PLATHE

Max-Planck-Institut für Polymerforschung, Ackermannweg 10, D-55128 Mainz, Germany
**E-mail: faller@mpip-mainz.mpg.de*

We investigate mutual local chain order in systems of fully flexible polymer melts in a simple generic bead-spring model. The excluded-volume interaction together with the connectivity leads to local ordering effects which are independent of chain length between 25 and 700 monomers, i.e. in the Rouse as well as in the reptation regime. These ordering phenomena extend to a distance of about 3 to 4 monomer sizes and decay to zero afterwards.

Keywords: Molecular Dynamics; Orientation Correlation; Polymer Melts.

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A STOCHASTIC CAGE MODEL FOR THE ORIENTATIONAL DYNAMICS OF SINGLE MOLECULES IN NEMATIC PHASES

DIEGO FREZZATO, GIACOMO SAIELLI, ANTONINO POLIMENO*†, and PIER LUIGI NORDIO

Dipartimento di Chimica Fisica dell'Università di Padova, Via Loredan 2, 35131 Padova, Italy
**E-mail: A.Polimeno@chfi.unipd.it*

A stochastic cage model for the orientational dynamics of a molecule in isotropic and nematic phases of a liquid crystal has been developed, following the methodology introduced in Refs. 1, 2. The model has been parameterized on the basis of statistical data obtained from the analysis of Molecular Dynamics (MD) simulations of a Gay-Berne mesogen and is based on the general assumption of a timescale separation between the fast inertial librational motion inside the instantaneous cage potential and the slow diffusive motion of the cage itself. The model is able to reproduce single molecule time correlation functions both for the angular momentum and the reorientation of the long molecular axis of the molecule. A complete description of the dynamics of a Gay-Berne particle is given with a single set of physical parameters, from a very fast (hundreds of femtoseconds) timescale up to a timescale of nanoseconds.

Keywords: Stochastic Models; Cage Dynamics; Liquid Crystals.

Footnotes:

†Corresponding author.

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SIMULATION OF NEMATIC FREE SURFACES

ENRIQUE DE MIGUEL* and ELVIRA MARTÍN DEL RÍO†

Departamento de Física Aplicada e Ingeniería Eléctrica, Universidad de Huelva, 21819 La Rábida (Huelva), Spain

**E-mail: demiguel@uhu.es*

†*E-mail: elvira@uhu.es*

Molecular dynamics and Monte Carlo methods are applied to study the liquid free surfaces in model liquid crystals. The simulation results suggest that the attractive interactions promote parallel alignment of the molecules at the nematic free surface in the Gay-Berne model, in agreement with theoretical predictions. A change in the orientation from planar to homeotropic is observed and explained in terms of a competing effect between attractive and repulsive interactions. Finally, the simulation results give clear evidence that the hard-core repulsions favor homeotropic orientation at the nematic free surface, in agreement with most theories.

Keywords: Computer Simulations; Liquid Crystals; Interfaces.

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