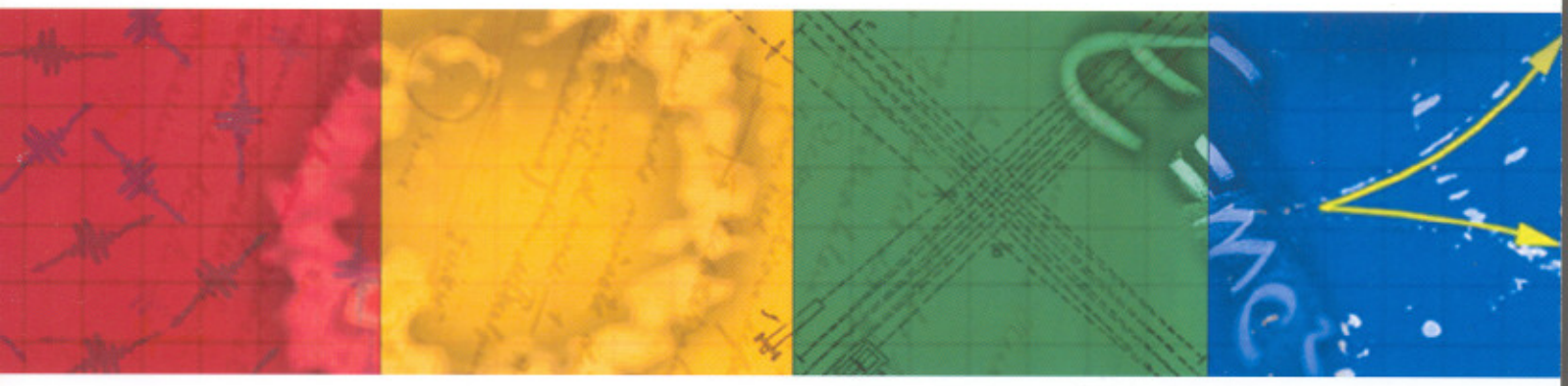
2006년 4월
제24권 제1호

한국물리학회

회보

BULLETIN OF THE KOREAN PHYSICAL SOCIETY



2006년 봄 학술논문발표회 및 제82회 정기총회

휘닉스파크

2006. 4. 20(목)~21(금)

KPS 사단법인 한국물리학회
The Korean Physical Society www.kps.or.kr

■ SESSION: F [FF1]
4월 20일(목), 14:30 - 16:00
휘닉스 2

FF-01(초) Parallel Replica Dynamics Investigation of Barrier Crossing Events for a Poly (Phenylene Ethynylene) (PPE) Synthetic Foldamer KUM Oyeon (*Com2MaC, Pohang University of Science and Technology.*) Synthetic molecules that exhibit secondary structure in solution have attracted considerable attention in recent years as potential templates in the production of regularly structured materials on a nanoscale. Recently, a series of novel synthetic PPE foldamers was reported to reversibly fold into well-defined helical structures. An understanding of atomistic folding mechanisms is highly useful in designing such molecules for use as structural templates and self-assembling nanomachines. Unfortunately, conventional computational techniques are fundamentally limited due to the long time scales needed to study the dynamics of folding. By employing parallel replica dynamics (PRD), a parallel algorithm in time domain, the simulation time scale can possibly be extended to that of real experiments, for example, the order of microsecond or millisecond. However, the effective implementation of PRD requires an efficient and accurate algorithm for detecting transitions as the molecular trajectories traverse from one state to another along the pathways of complex system. At the conference, I am going to show the different atomistic transition mechanisms of PPE using PRD simulations.
*This work was supported, in part, by the SRC/ERC program of MOST/KOSEF (#:R11-1999-054).

FF-02(초) Boundary Conditions in Nanoflows JUNG Youngkyun, LEE Jysoo(*KISTI, Supercomputing Center.*) Molecular dynamics simulations are used to study the boundary conditions at a fluid-solid interface and a nanometer-size solid sphere in a rotating fluid-filled cylindrical nanochannel. Our attention is given to the effects of varying the wetting properties of the fluid and the solid particle. We will also show slip length for the flow in a rotating cylindrical tube as a function of the wetting parameter.

FF-03(초) Effective Hamiltonian for the Thermodynamic Glass Transition 여 준현, MOORE M. A.[1] (*건국대학교, 물리학과. [1]University of Manchester, School of Physics and Astronomy.*) We set up an effective Hamiltonian describing supercooled liquids near their thermodynamic glass transition using a replica formulism. The resulting Hamiltonian is equivalent to that for an Ising spin glass in a magnetic field. Results taken from the droplet picture of spin glasses are then used to provide an explanation of the main features of fragile glasses.

FF-04(초) Modelling Collective Behavior of Molecules in Nanoscale Direct Deposition Processes 이남경, 홍 승훈[1](*세종대학교 물리학과. [1]서울대학교 물리학부.*) We present a theoretical model describing the collective behavior of molecules in direct deposition processes such as dip-pennanolithography. We show that intermolecular interactions combined with non-uniform substrate-molecule interactions can produce various shapes of molecular patterns including fractal-like structures. Computer simulations reveal circular and star-like patterns at low and intermediate densities of preferentially-attractive surface sites, respectively. At largedensity of such surface sites, the molecules form atwo-dimensional invasion percolation cluster. Previous experimental results showing anisotropic patterns of various chemical and biological molecules correspond to the star-like regime.

FF-05(초) Stochastic Coherence in Globally Coupled Inhibitory Neurons LIM Woochang, KIM Sang-Yoon[1](*아주대, 의과학연구소. [1]강원대, 물리학과.*) We study the collective dynamics in a large population of Morris-Lecar neurons with a global non-instantaneous inhibitory coupling. When the inhibitory synaptic coupling has appropriately large strength and decays slowly, coherence of noise-induced firings is found to occur. By varying the noise intensity, such stochastic coherence is investigated in terms of the global output signal (i.e., the ensemble-averaged membrane potential) which plays the role of the order parameter. This order parameter is maximized at some optimal noise strength. For the coherent case, the global output signal exhibits a collective oscillation, and its dynamical properties are also analyzed. To measure the degree of (noise-induced) stochastic coherence, we introduce a coherence measure by considering both the fraction of firing neurons and the degree of contribution of local spikings to the global spiking. As such spiking measure is in-