CPP 36: Particulate Matter: From microscopic interactions to collective motion (joint session DY/CPP)

Time: Tuesday 14:00–15:45   Location: EB 107

CPP 36.1 Tue 14:00 EB 107

Onset of anomalous diffusion in colloids confined to quasi-monolayers — •MARTIN OETTEL[1], JOHANNES BLEIBEL[1], and ALVARO DOMINGUEZ[2] — [1]Institut für Angewandte Physik, Universität Tübingen — [2]Fisica Teorica, Universidad de Sevilla

It has been recently shown that a colloidal monolayer, e.g., formed at a fluid interface or by means of a suitable confining potential, exhibits anomalous collective diffusion: diffusion becomes accelerated as signalled by a $1/k$–divergence of the wavenumber–dependent collective diffusion coefficient. This is a consequence of the hydrodynamic interactions mediated by the three-dimensional (3D) ambient fluid when the particles are confined to reside on a two-dimensional (2D) manifold. We study theoretically and with numerical simulations the crossover from normal to anomalous diffusion as the particles are, in real systems, confined by a 3D external potential and thus have the possibility to fluctuate out of the 2D manifold, thus forming a quasimonolayer. In essence, we always find anomalous diffusion on lateral length scales larger than the confinement width.

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Microrheology in hard colloids with large tracers — •ANTONIO M. PUERTAS[1], FRANCISCO ORTS[2], GLORIA ORTEGA[2], and ESTER M. GARZON[2] — [1]Dpt. of Applied Physics, Univ. of Almeria, Almeria, Spain — [2]Dept. of Informatics, Univ. of Almeria, Agrifood Campus of Int. Excell., ceiA3, Almeria, Spain

Microrheology has become recently in a powerful technique to study the dynamics of a system in microscopic scales. A colloidal tracer is introduced in the host system, and its dynamics is monitored. When an external force acts on the tracer, the system goes out of equilibrium probing the linear regime for small forces, and entering the non-linear regime for large ones. A colloidal bath of hard spheres is probably the simplest example. Several theory models have been developed, tested by simulations, but typically these restrict to tracers of the same size as the bath particles.

Here, we present simulation results of the dynamics of a tracer pulled with a constant force in a colloidal bath. The tracer size, a_t, is larger than the bath particles, size a, up to $a_t = 5a$. Important finite size effects appear, particularly for large tracers, which have been studied and compared with predictions from hydrodynamics for the bath. Due to the massive computational demand, the simulations were computed on a multiGPU cluster and a genetic algorithm was designed to optimize the performance. The dynamics of the tracer, providing the friction coefficient with the bath and the effects of the bath (density fluctuations, and strain field) are studied for small forces. The theoretical limit of an infinite tracer, $a/a_t \to 0$, and small forces, is checked.

CPP 36.3 Tue 14:30 EB 107

Efficient simulation of anisotropic particles using collective Monte Carlo moves — •MARCO KLEMENT and MICHAEL ENGEL — Institute for Multiscale Simulation, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

Hard anisotropic particles are a classical model for the influence of shape on the thermodynamic behaviour of particulate matter. Examples are the phase diagram of liquid crystal formers and the prediction of crystal structures for polyhedral nanocrystals [1]. Here, we investigate the speed-up of hard polyhedra Monte Carlo simulations by using collective chain moves [2]. Our implementation relies on analytically detecting sweep collisions with an improved version of the Minkowski portal refinement algorithm. We validate our method by calculating equations of state and studying self-assembly phenomena.

[1] M.A. Boles, M. Engel, D.V. Talapin, Chem. Rev. 116, 11220-11289 (2016).

[2] E.P. Bernard, W. Krauth, D.B. Wilson, Phys. Rev. E 80, 056704 (2009).

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Stochastic Nature of Granular Tribocharging — •JAN HAEBERLE[1], ANDRÉ SCHELLA[2], MATTHIAS SCHRÖTER[2], MATTHIAS SPERL[1], and PHILIP BORN[1] — [1]Deutsches Zentrum für Luft- und Raumfahrt, Köln, Deutschland — [2]MPI Dynamics and Self-Organization, Göttingen, Germany

Triboelectric charging of granular media has important consequences for the bulk behaviour. Effects such as powder flowability or cluster formation due to charging are everyday experiences [1]. Triboelectric charging has also been linked to segregation [2] and suggested as a tool for structure formation in granular media [2,3]. Recently, the stochastic nature of the triboelectric charging process has become apparent [4]. To further investigate the stochastics of tribocharging, we have studied the distribution resulting after a tribocharging event in a custom-made Faraday cup setup. We measure non-Gaussian asymmetric charge distributions. We find, that we can describe the measured distributions by a model combining a distinct stochastic charging and stochastic discharging process.

[1] Duran, J., Sands, Powders, and Grains, Springer, New York (2000) [2] Schella, A., Herminghaus, S. & Schröter, M., Soft Matter 13, 394-401 (2017). [3] Cademartiri, R. et al., Soft Matter 8, 9771 (2012). [4] Apodaca, M. M., Wesson, P. J., Bishop, K. J. M., Ratner, M. A. & Grzybowski, B. A., Angewandte Chemie 122, 958-961 (2010).

CPP 36.5 Tue 15:00 EB 107

Universal hidden order in amorphous cellular geometries — •MICHAEL A. KLATT[1], JAKOV LOVRIĆ[2,3], DUYU CHEN[4], SEBASTIAN C. KAPFER[5], FABIAN M. SCHALLER[5,1], PHILIPP W. A. SCHÖNHÖFER[3,5], BRUCE S. GARDINER[3], ANA-SUNČANA SMITH[2,5], SALVATORE TORQUATO[4,6], and GERD E. SCHRÖDER-TURK[3,5] — [1]KIT, Institute of Stochastics, 76049 Karlsruhe, Germany — [2]Division of Physical Chemistry, Ruder Bošković Institute, Zagreb, Croatia — [3]Murdoch University, School of Engineering and Information Technology, 90 South St, Murdoch WA 6150, Australia — [4]Department of Chemistry, Princeton University, New Jersey 08544, USA — [5]Institute for Theoretical Physics, FAU, 91058 Erlangen, Germany — [6]Department of Physics, PRISM, PACM, Princeton University, New Jersey 08544, USA

Starting from an amorphous partitioning of space into cells, we iteratively optimize the "centrality" of the cells, minimizing the so-called Quantizer energy. The energy landscape is replete with local minima to which the system converges despite the existence of lower-energy crystalline configurations. Irrespective of the level and type of disorder in the initial configurations, the tessellations converge to the same amorphous state, as measured by the same structure factor and energy distributions. The final disordered configurations exhibit an anomalous suppression of long-wavelength density fluctuations, known as hyperuniformity. For systems related to the Quantizer problem, such as self-assembled copolymeric phases, our findings suggest the possibility of stable disordered hyperuniform phases.

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Relaxation of hydrogen bond network in water subject to E-field — •ANDREAS BAER[1], ZORAN MILICEVIC[1,2], DAVID MATTHEW SMITH[2,3], and ANA-SUNCANA SMITH[1,2] — [1]PULS Group at the Institute for Theoretical Physics and EAM, FAU Erlangen-Nürnberg, Germany — [2]Division of Physical Chemistry, Institute Ruđer Bošcović, Zagreb, Croatia — [3]Computer Chemistry Center, FAU Erlangen-Nürnberg, Germany

Most of the amazing properties of liquid water stem from the fluctuations in the uninterrupted network of hydrogen-bonded molecules.[1] One such phenomena is the splitting of transport coefficients in an electric field, which despite the enormous technological implication, is an effect not yet understood from the microscopic point of view. We address this problem by simulating pure water in a uniaxial E-field under ambient conditions using the GROMACS framework.[2] After quantifying the translational and orientational dynamics of water molecules, characteristic, anisotropic timescales for the reordering of hydrogen bonds are retrieved. A novel relaxation process occurring on the picosecond timescale is detected, and unambiguously associated with cooperative rotations of multiple hydrogen-bonded molecules that induce a slow relaxation of components of the macroscopic shear viscosity that are parallel to the field direction.[3] [1] Luzar, A.; Chandler, D. Nature 1996 379, 55-57. [2] Milicevic Z., Marrink S. J., Smith A.-S., Smith D. M. J. Mol Mod 2014 20, 2359 [3] Milicevic Z., Baer A., Smith D. M., Smith A.-S., PRX submitted

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In-cage dynamics of molecular hydrogen in clathrates hydrates as function of the confinement size — ●Margarita Russina — Helmholtz Zentrum Berlin für Materialied und Energie, Hahn-Meitner Platz 1, 14109 Berlin

To understanding the criteria governing the molecular mobility in confinement we have studied in-cage dynamics of confined molecular hydrogen as a function of confinement size. We used nanopores ice based clathrate with nanocages of two different dimensions of 0.75 and 0.946 nm, which are particularly suitable model systems since the interactions between the clathrate framework and H2 are of the same hydrophobic nature in both cages. We have found that by varying the size of the pore by only 20 % in the effective radius we can modify the diffusive mobility of confined hydrogen in both directions, i.e. both reducing and enhancing mobility compared to the bulk. In the smaller cages of clathrate hydrates with a mean size of 0.795 nm we observe strong hydrogen localization in the cage center even at temperatures up to 200K. Moderate increase of the confinement to 0.946 nm leads to the onset of jump diffusion between tetrahedrally shaped sorption sites in large cages with separation length of about 2.79 Å already at T=10 K, where bulk hydrogen is frozen at ambient pressure. The observed difference in mobility between small and large cages can be understood as a dimensional phenomenon caused by the modulation of cage potentials as a function of the cage size.