

CPP 45: Modeling and Simulation of Soft Matter IV

Time: Thursday 15:00–16:30

Location: H 0111

CPP 45.1 Thu 15:00 H 0111

Multiscale simulations to understand pairing and stacking at the origin of life — ●LAURIE STEVENS¹, RICCARDO MARTINA², ALBERTA FERRARINI², and MARIALORE SULPIZI¹ — ¹Physics Department, Ruhr Universität Bochum, Germany — ²Chemical Science Department, Università di Padova, Italy

Our research focus on life's beginnings by examining nucleotide interactions, a critical point in RNA formation. Using Molecular Dynamics, we aim to understand how self-assembly of these components can promote the synthesis of long polynucleotides. However, due to the system's complexity and scale, traditional ab initio methods are too slow for our targeted timescales of several nanoseconds.

To bypass these limitations, we turn to the Machine Learning approach, employing DeepMD. We train neural networks potentials (NNPs) to mimic the intricate behaviours of nucleotides. As a first step we consider a single AMP molecule in water, where we aim to reproduce the complex free energy landscape as function of the relevant degrees of freedom.

The trained NNPs are able to accurately reproduce the solvation structure around the different chemical groups, as well as the conformational changes associated to the torsional angles around the sugar and the phosphate groups.

CPP 45.2 Thu 15:15 H 0111

Microscopic insights on the puzzling saddle-splay elasticity of nematics — ●DAVIDE REVIGNAS^{1,2} and ALBERTA FERRARINI¹ — ¹Department of Chemical Sciences, Padua, Italy — ²Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

The elasticity of a nematic liquid crystal is commonly understood in terms of the Frank deformation free energy which involves splay (K11), twist (K22) and bend (K33) elastic constants. There exists, however, a fourth term commonly referred to as the saddle-splay deformation mode, which is associated to the elastic constant K24.

Recent experiments on confined chromonic liquid crystals revealed a twisted ground state which has been ascribed to $K24 > K22$. This would violate one of the Ericksen inequalities for the stability of the nematic uniform state. In general, experimental estimates of K24 are difficult to obtain and only few, sometimes contradictory data are available. Moreover, the estimation of K24 is a challenging task also for microscopic theories of elasticity; indeed, the very possibility of an unambiguous calculation of this quantity starting from a microscopic model has been questioned.

Here we will present the results of the calculation of the full set of elastic constants, including K24, for simple hard rods in the framework of Onsager theory for nematics. Such results enable us to discuss the possible origin of a twisted ground state for this simple model of nematics, in spite of the absence of microscopic chirality.

CPP 45.3 Thu 15:30 H 0111

Scaling Properties of Tree-like Regular Polymeric Fractals — ●RON DOCKHORN¹ and JENS-UWE SOMMER^{1,2} — ¹Leibniz-Institut für Polymerforschung Dresden e.V., D-01069 Dresden, Germany — ²Technische Universität Dresden, Institut für Theoretische Physik, D-01069 Dresden, Germany

This study compares regular polymeric Vicsek- and T-fractals with dendrimers using theory and simulations. While all structures show exponential growth in the number of monomers and terminal groups, their structural properties differ significantly. Computer simulations are conducted to analyze the scaling properties of these tree-like self-similar polymeric fractals, using the Bond-Fluctuation-Model with the Metropolis method and the parallelized Wang-Landau algorithm. The radius of gyration, scattering intensity, and θ -point of these systems are examined to study the coil-globule transition of the polymeric fractals. A mean field theory is applied to determine the scaling exponent in different solvent conditions, which is found to be in fair agreement with the simulation data. A transition from almost linear chain behavior to a spherical shape is observed, and this can be controlled by the inherent functionality of the building blocks. Consequently, polymeric fractals can serve as an alternative to dendrimers in the category of hyperbranched polymers.

CPP 45.4 Thu 15:45 H 0111

Modeling phenolic (aero)gels: A computational approach — ●HEMANGI PATEL¹, MATTHEW ADDICOAT², BARBARA MILOW^{1,3}, and AMEYA REGE^{1,4} — ¹German Aerospace Center (DLR), Institute of Materials Research, Department of Aerogels and Aerogel Composites, 51147 Cologne, Germany — ²Nottingham Trent University New Hall Clifton Campus — ³Institute of Inorganic Chemistry, University of Cologne, 50939 Cologne, Germany — ⁴School of Computer Science and Mathematics, Keele University, Staffordshire, ST 5BG, United Kingdom

Phenolic aerogels, comprising over 90% gaseous volume, exhibit low density, large surface areas, high pore volume, and minimal thermal conductivity. Derived mainly from resorcinol-formaldehyde (RF) polycondensation, these aerogels find diverse applications. The sol-gel chemistry significantly influences their properties, demanding a bottom-up understanding. Although less explored, molecular design holds immense potential to enhance structure-property relations and accelerate aerogel development. This involves optimizing conditions (temperature, pH, precursor concentrations) and employing data-driven approaches. This work illustrates a novel approach to RF gelation design at the molecular level, simulating the reaction chemistry for approximately 50,000 RF monomer molecules within a proposed framework. Characterization includes varying densities, pore wall curvature, voids, pore-size distributions, and surface areas. This strategy aims to propel development of new molecularly-architected aerogel systems by combining experimental optimization and data-driven simulations.

CPP 45.5 Thu 16:00 H 0111

Impact of local structure variations on air flow through porous sheets — ●KARIN ZOJER¹, EKATERINA BAIKOVA¹, MATTHIAS NEUMANN², PHILLIP GRÄFENSTEINER², PETER LEITL³, ANDONI RODRIGUEZ³, ANDRE HILGER⁴, INGO MANKE⁴, ULRICH HIRN¹, and VOLKER SCHMIDT² — ¹Graz University of Technology, Graz, Austria — ²Ulm University, Ulm, Germany — ³bionic surface technologies, Austria — ⁴Institute of Materials, Helmholtz Zentrum Berlin, Berlin, Germany

Predicting the rapid transport of gases through inhomogeneous porous layers is difficult because the flow tends to be dominated by a few effective paths, which differ from the most frequently occurring paths of the structure. By looking at the microstructure, is it possible to predict these most effective transport pathways, assuming that all local variations are known? What combination of local structural properties favors these pathways? We combine computational fluid dynamics and pore network pore network simulations with a copula-based property-pair dependence analysis to address these questions for air transport through two model materials. These materials are paper sheets, before and after uniaxial compression, whose microstructural variations are fully known from μ -CT 3D imaging. Compression converts large variations in sheet thickness into large variations in density and is therefore expected to localize the air flow and alter the relevant pathways.

CPP 45.6 Thu 16:15 H 0111

Solubility of NaCl in Aqueous Solution using Kirkwood-Buff Integration — ●ABHISHEK CHATTOPADHYAY, VARUN MANDALAPARTHY, and NICO F. A. VAN DER VEGT — Department of Chemistry, Technical University Darmstadt, 64287 Darmstadt

Aqueous electrolyte solutions are ubiquitous in both chemical and biological environments. While molecular simulations are well suited to study these systems, empirical force fields for ion-ion and ion-water interactions are frequently not sufficiently accurate. The aqueous solubility of electrolytes is particularly sensitive to interactions in solution and thus a useful target in model-validation studies. In this work, we used the chemical potential route to calculate the solubility of NaCl using Kirkwood-Buff (KB) integration for the chemical potential of NaCl in the aqueous phase combined with Einstein integration for the solid phase. We consider the full charge Joung-Cheatham ion model combined with SPC/E water as our model system. The effect of ensemble and finite-size corrections applied to the radial distribution functions and KB integrals on the solubility will also be discussed. The KB integration method provides a computationally efficient and accurate route and can be used to compute salt solubility using ion forcefields developed in our research group which incorporate softer ion-water re-

pulsion than the conventional Lennard-Jones potential[1].

[1] M. P. Bernhardt, Y. Nagata, and N. F. A. van der Vegt. J. Phys.

Chem. Lett., 13(16):3712-3717, 2022.