CPP 60: Focus: Two Dimensional Functional Materials II

Time: Thursday 15:00–16:00 Location: H51

Invited Talk CPP 60.1 Thu 15:00 H51

Evolution of mono- and bilayer graphene in chemical vapor deposition and the thinnest feasible porous membranes for ultimate mass transport — •Hyung Gyu Park — Nanoscience for Energy Technology and Sustainability, Department of Mechanical and Process Engineering, ETH Zurich, Zurich, Switzerland

Graphene as the seminary 2D material poses great potential in many applications for its electronic, thermal, optical and mechanical properties unique and superior to other materials. Today a majority of technological applications use graphene produced via chemical vapor deposition and transferred onto destination substrates. This talk will present overview and our results of the growth of mono- and bilayer graphene on copper foils, leading to a discussion on kinetics, energetics and mechanisms of the graphene formation on copper. An interesting demonstration of the thinnest feasible porous membranes by use of our graphene illustrates the promises that 2D materials pose. Gas transport across the 2D porous membrane shows a wide range of transport mechanisms from free molecular to transition to continuum dynamics. Water transport measurement agrees well with a capillarity effect and an orifice theory. Discussion on technological implications will follow.

CPP 60.2 Thu 15:30 H51

Cluster Formation of Carbon Nanotubes in Lipid Bilayers — •Martin Vögele, Jürgen Köfinger, and Gerhard Hummer — Max-Planck-Institut für Biophysik, Frankfurt am Main

We investigate the clustering behavior of open-ended carbon nanotubes in lipid membranes by means of atomistic and coarse-grained molecular dynamics simulations. On the atomistic scale, we gain insight in the interactions of the nanotubes with lipids and with each other. The coarse-grained scale allows us to simulate the clustering of one hundred nanotubes for tens of microseconds. In our simulations, we vary parameters such as tube length and tube diameter. We also consider different functionalization of the carbon nanotubes, as well as different lipid compositions of the membrane.

We find that the up-right carbon nanotubes induce strong order in the lipids, which form ring-like structures around the tubes. Nanotubes quickly form clusters in which neighboring nanotubes are separated by a single layer of lipids, although free energy calculations suggest that direct nanotube contacts are more favorable. Only when we reduce lipid-nanotube interactions significantly, we observe the spontaneous formation of direct contacts. Thus, depending on the lipid-nanotube interactions, clusters can be kinetically trapped, which has important implication for large-scale applications.

CPP 60.3 Thu 15:45 H51

Graphitic carbon nitrides as graphene complements: new insights and challenges — •Christoph Merschjann — Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin

"Graphitic" carbon nitride (CN) polymers are currently studied all over the world, mainly for photocatalytic processes like metal-free solar water-splitting, but also for solid-state lighting, hybrid photovoltaics, and organic electronics in general. Bearing its name due to a two-dimensional polymeric structure, the CN material class shows several fascinating properties, such as tunable optical band gap in the UV-VIS-IR range, comparably easy synthesis processes, and high chemical and thermal stability.

Just recently we could deduce the charge carrier mobility from transient fluorescence measurements, showing that the CN material class comprises reasonable candidates for optoelectronic applications. Moreover, we found that charge transport is mainly confined to channels perpendicular to the two-dimensional structure [1]. The materials thus complement graphene, possibly opening the way for novel applications.

The talk will give an overview of the latest opto-electronic physical findings in different CN materials as well as a discussion of the challenges of such measurements in optically scattering samples.

[1] C. Merschjann et al., *Advanced Materials* **2015**, DOI: 10.1002/adma.201503448