

IAP Seminar



Jürgen Schnack

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Tuesday, 22th November 2022, 16:00 s.t.
TU Wien, Institut für Angewandte Physik, E134
1040 Wien, Wiedner Hauptstraße 8-10
Yellow Tower "B", 5th floor, SEM.R. DB gelb 05 B





Theoretical formation of carbon nanomembranes under realistic conditions using classical molecular dynamics

Carbon nanomembranes made from aromatic precursor molecules are freestanding nanometer-thin materials of macroscopic lateral dimensions. Although produced in various versions for about two decades, not much is known about their internal structure. Here we present a systematic theoretical attempt to model the formation, structure, and mechanical properties of carbon nanomembranes using classical molecular dynamics simulations. We find theoretical production scenarios under which stable membranes form. They possess pores as experimentally observed. Their Young's modulus, however, is systematically larger than experimentally determined.

Alternative approaches as well as an outlook how to advance our theoretical understanding are provided.

Jürgen Schnack is a University Professor at Bielefeld University working in theoretical condensed matter physics mainly on problems of quantum magnetism. He studied physics in Dresden and Darmstadt and wrote his Diploma and Ph.D. theses on problems of nuclear few-body physics. During his habilitation at Osnabrück University he shifted his focus to molecular magnetism. He received the Hans-Mühlenhoff Prize for excellent habilitations and was appointed at Bielefeld University in 2007.

All interested colleagues are welcome to this seminar lecture (45 min. presentation followed by discussion).

Friedrich Aumayr (LVA-Leiter)

R.A. Wilhelm (Seminar Chair)