IAP Seminar

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Tuesday, 8th October 2019, 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

Ab initio simulation of correlated electrons: From graphene nanoribbons to warm dense matter

The Coulomb interaction between electrons gives rise to interesting collective behavior that is manifest in many systems around us – from astrophysics to the nanoscale. For theoretical physics, strong Coulomb correlations are a challenge because familiar models such as ideal gas, Hartree-Fock or perturbation theory break down. The alternative are computer simulations that have seen dramatic progress in recent years. I will present two examples of recent work. The first are finite graphene-type structures (nanoribbons, heterostructures) which we model using nonequilibrium Green functions. The results include the stopping power of charged projectiles and the formation of topological edge states. The second example is „warm dense matter“ – highly compressed and excited matter on the border between solid and plasma. Here I outline new quantum Monte Carlo methods that have allowed us to compute the thermodynamics properties, the dynamic structure factor and the electron plasmon dispersion from first principles.

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Michael Bonitz is a professor of theoretical physics at CAU Kiel where he holds the chair for Statistical Physics and works on computer simulations for plasmas and condensed matter systems. He received a physics diploma from Lomonosov University Moscow, the PhD and habilitation from Rostock University, and did postdoctoral research at the University of Arizona, Tucson. He has been a visiting professor at the University of Florida, Gainesville, is a recipient of the Gustav-Hertz prize of the German Physical Society, a fellow of the American Physical Society and Doctor honoris causa of the Russian Academy of Sciences. URL: http://www.theo-physik.uni-kiel.de/bonitz

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

Friedrich Aumayr
(LVA-Leiter)