Novel Materials Based on Carbon nanostructures

Alexander Kaiser[a], Frank Hagelberg[b],

[a]Institut für Ionenphysik, Leopold-Franzens Universität, Innsbruck, Austria

[b]***Department of Physics and Astronomy, East Tennessee State University, Johnson City, TN 37614, USA***

Carbon nanostructures display a broad range of properties which can be tuned to match an equally broad variety of actual or potential applications. This presentation deals with novel materials based on zero-, one-, and two-dimensional nanostructures.

Specifically, we will emphasize single-walled carbon nanotubes (SWCNTs) of the zigzag type. These species are known to turn magnetic upon dimensional reduction to axially confined units. Recent plane-wave density functional theory (PL-DFT) simulations have extended these elements to cross-linked carbon nanotubes (CLCNTs), composed of three SWCNTs which are of interest for both nanomechanics and nanoelectronics. Various CLCNT models, differing from each other by the structure of the contact regions of the three SWCNT constituents, will be explored in terms of their geometric, electronic, and magnetic properties. Various magnetic phases, as obtained by combining finite SWCNTs in ferromagnetic (FM) or antiferromagnetic (AFM) coordination, are distinguished. These phases are shown to depend on the contact region geometry which defines the order of their stabilities. A wide variety of magnetic networks, with potential applications in spintronics, can be built from these nanosystems.

A further focus of our presentation will involve novel phases consisting of two-dimensional arrays of fullerenes deposited on metal surfaces through a process of controlled self-assembly. We will discuss energy criteria that determine the formation of adsorbate-induced vacancies following the self-assembly of the adsorbates on clean surfaces. These mechanisms will be exemplified by C_{60} in contact with Al(111), Au(111), and Be(0001) surfaces, making allowance single, triple, and septuple atom pits. Modes of vacancy-adatom formation that govern the adsorption processes will be highlighted.