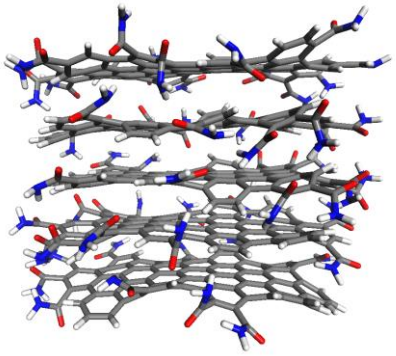
The Electronic Structure of Amorphous and Graphitic Carbon Nanoparticles

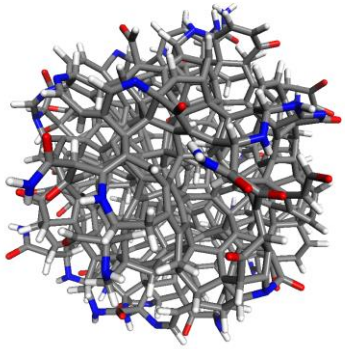
Johannes T. Margraf,[1,2] Volker Strauß,[2] Dirk M. Guldi,[2] Timothy Clark[1]

[1]*Computer Chemie Centrum, Nägelsbachstr. 25, 91052 Erlangen*

[2]*Physikalische Chemie I, Egerlandstr. 3, 91058 Erlangen*

Carbon nanodots (CNDs) can easily be synthesized from small molecules and feature interesting properties, most prominently strong, tunable photoluminescence and high water solubility. The structure of these materials is difficult to study experimentally because the particles are usually quite polydisperse. Additionally, CNDs consist exclusively of light elements (C,N,O) with low scattering cross-sections towards electron and X-ray radiation, limiting the use of many important characterization methods (e. g. TEM, XRD).





We have developed two distinct structural models for CNDs. On the one hand, we constructed heavily functionalized graphene/graphite particles. On the other hand, we considered amorphous carbon spheres with relatively low density, which feature a considerable amount of sp^2 atoms. In this case the role of nitrogen impurities was also investigated. To study the geometry and electronic structure of these models (which consist of thousands of atoms), we relied on the massively parallel semi-empirical molecular orbital theory program EMPIRE.[1]

[1] Clark, T.; Hennemann, M. EMPIRE; Friedrich-Alexander- Universität Erlangen-Nürnberg: Erlangen, Germany, 2011.