Understanding the structure of disordered carbons through calculations of NMR spectra

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Disordered carbons are used in several applications, including as electrodes for supercapacitors, where their capacitance has been shown to dramatically increase at nanometric pore sizes. An in-depth understanding of the atomic-scale structure in these materials can lead to the development of devices having an improved performance and the optimization of fabrication protocols. NMR spectroscopy is a prominent method for the characterization of such materials, however it is still not completely clear how the spectral characteristics correlate to the different structural motifs in disordered carbons. In this work we employ a series of DFT calculations of isotropic NMR shieldings on disordered carbon systems with varying densities in order to obtain more insight on the response of the carbon atoms. We report on specific topological effects on the shieldings, such as the response of under- and over-coordinated atoms, or their variation with respect to the nearest neighbour distances or angular distributions. We also correlate the results with the meso- and macro-scale structure of the disordered carbons under study, more specifically the ring distribution and the system density.