

MAR14-2013-020709

Abstract for an Invited Paper  
for the MAR14 Meeting of  
the American Physical Society

### **Novel Carbons as Electrodes for Electrical Energy Storage**

RODNEY S. RUOFF, The University of Texas at Austin

In this talk I will speculate about directions for carbon materials as the electrode(s) in EES systems such as ultracapacitors and Li ion batteries. Perhaps the penultimate electrode material for ultracapacitors (based on charge storage by electrical double layer capacitance, EDLC) would be a “negative curvature carbon” (NCC, akin to the Schwartzite structures) with atom thick walls, and possibly substitutionally doped with, e.g., N atoms in case the all-carbon structure were limited by quantum (i.e., intrinsic) capacitance. Such an NCC would have a distribution of pore sizes that would likely (for optimal performance) span “mesoscale” and “microscale” pores, which in the parlance of porous materials means pores “above 2-3 nanometers” and pores “below about 2 nanometers,” respectively. Making such materials offers exciting challenges for materials chemists/synthetic chemists, and to date only the “basic” Schwarzite structures (ideal crystals studied by DFT with periodic boundary conditions and relatively simple unit cells) have been modeled in terms of properties such as their electronic states and in some cases, potential as all carbon ferromagnets. I identified the NCCs as candidates for EES for ultracapacitors, in a paper published in *Science* in 2011 with coauthors. We made an aperiodic carbon that had atom thick walls and surface areas as high as 3200 m<sup>2</sup>/g, along with “good” powder electrical conductivity, high carbon content, and apparently close to 100% trivalently bonded carbon in the walls of this very porous carbon. We have learned in one set of experiments, as published in *Energy and Environmental Science*, that doping with N atoms can increase the EDLC, which we suggest could be a consequence of limiting quantum capacitance in the all-carbon analogue.