Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Hydroxyl-decorated Graphene Systems: Organic metal-free Ferroelectrics, Multiferroics, and Proton battery Cathode Materials
MENGHAO WU, Department of Physics, Virginia Commonwealth University, Richmond, VA 23284, J.D. BURTON, EVGENY TSYMBAL, Department of Physics, University of Nebraska, Lincoln, NE 68588, XIAO CHENG ZENG, Department of Chemistry, University of Nebraska, Lincoln,NE 68588 , PURU JENA, Department of Physics, Virginia Commonwealth University, Richmond, VA 23284, PROF.JENA'S GROUP TEAM, PROF.BURTON'S GROUP TEAM, PROF.TSYMBAL'S GROUP TEAM, PROF.ZENG'S GROUP TEAM — Through density-functional-theory calculations we show that hydroxylized graphene systems are ideal candidates for light-weight organic ferroelectric materials with giant polarizations. For example, the polarization of semi-hydroxylized graphane and graphone as well as fully hydroxylized graphane are, respectively, 41.1, 43.7, 67.7 μC/cm^2, much higher than any organic ferroelectric materials known to date. In addition, hydroxylized graphone is multiferroic due to the coexistence of ferroeletricity and ferromagnetism. Zigzag graphene nanoribbons decorated by hydroxyl groups also exhibit ferroelectric properties with a large polarization of 27.0 μC/cm^2. Moreover, proton vacancies at the end of ribbons can induce large dipole moments that can be reversed by both hopping of protons and rotation of O-H bonds under an electric field. These materials have the potential as high-capacity cathode materials with specific capacity six times larger than lead-acid batteries and five times that of lithium-ion batteries.

Menghao Wu
Department of Physics, Virginia Commonwealth University,
Richmond, VA 23284

Date submitted: 25 Oct 2012 Electronic form version 1.4