SUPPORTING INFORMATION

Hydration Peculiarities of Graphene Oxides with Multiple Oxidation Degrees

Antenor Neto¹, Vitaly V. Chaban,² and Eudes E. Fileti³

¹ Centro de Ciências Naturais e Humanas, Universidade Federal do ABC, 09210-170, Santo André, SP, Brazil.

² P.E.S., Vasilievsky Island, Saint Petersburg, Russian Federation.

³ Instituto de Ciência e Tecnologia, Universidade Federal de São Paulo, 12231-280, São José dos Campos, SP, Brazil.

*Corresponding author. e-mail: fileti@gmail.com. Fax: +55 12 3924 9500

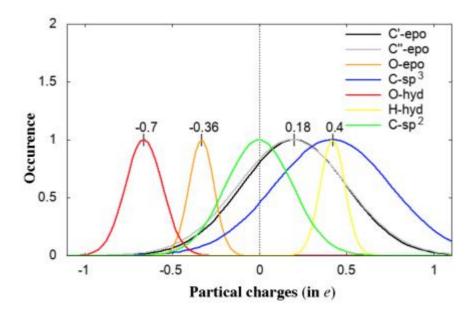


FIGURE S1: Distributions and average charges obtained on all similar atoms for each of the graphene oxides.

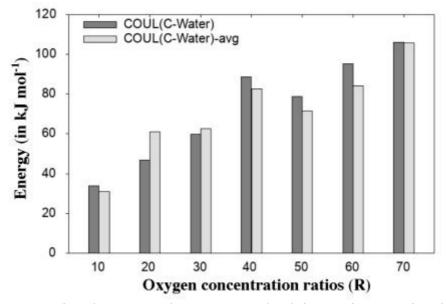


FIGURE S2: Comparison between carbon-water Coulomb interaction energies obtained with both charge sets; CHELPG (dark bars) and average charges (light bars).

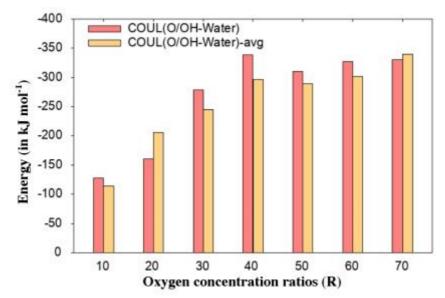


FIGURE S3: Comparison between O/OH-water Coulomb interaction energies obtained with both charge sets; CHELPG (dark bars) and average charges (light bars).

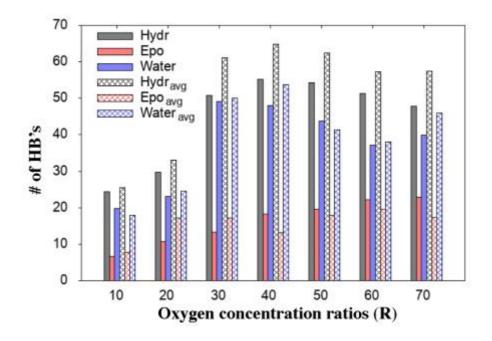


FIGURE S4: Average number of hydrogen bonds obtained with both charge sets; CHELPG (solid bars) and average charges (traced bars).

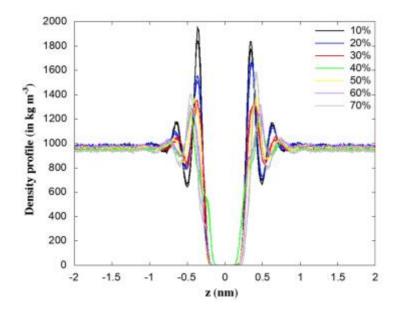


FIGURE S5: Profile of mass density for each oxygen concentration ration.