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Multiphonon Raman spectroscopy and optical properties for graphene-family nanomaterials: Role of surface functionality on electronic and phonon density of states. B. EVANS, A. HENSON, R. MEEK, Western Kentucky University, Physics Dept. Bowling Green, KY, N. DIMAKIS, Department of Physics, The University of Texas-Rio Grande Valley, TX 78539 , S. GUPTA, Western Kentucky University, Physics Dept. Bowling Green, KY — We report optical and lattice vibrational properties of a range of graphene-family nanomaterials using UV-visible absorption, photoluminescence excitation, PLE and micro-Raman spectroscopy (RS) techniques. Various functionalized graphene nanomaterials include few layer graphene oxide, reduced graphene oxide, graphene quantum dots and three-dimensional graphene aerogel scaffolds and their nitrogenated counterparts. RS provides lattice dynamical nanoscale structural characterization revealing collective atomic/molecular motions and localized vibrations. The role of oxygen epoxy (C-O-C, carbonyl, C=O) and nitrogen (pryridinic and graphitic/pyrrolic) functionalities and corresponding bonding configurations with quantum size effects are emphasized in view of understanding physico-chemical properties for biosensing and water desalination. While first- and second-order phonon modes are analyzed in terms of Raman intensity, band position (intrinsic mechanical strain) and intensity ratio (structural disorder, number defect density), distinct localized π electronic states were found in PLE spectra reflecting carbon atoms around oxygenated and nitrogenated species. The origin of these states is discussed based on experimental findings and DFT exemplifying structural evolution.

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