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Controllably Inducing and Modeling Optical Response from Graphene Oxide NICHOLAS LOMBARDO, Central Conencticut State University, ANTON NAUMOV, Texas Christian University — Graphene, a novel 2-dimensional sp^2-hybridized allotrope of Carbon, has unique electrical and mechanical properties. While it is naturally a highly conductive zero band gap semiconductor, graphene does not exhibit optical emission. It has been shown that functionalization with oxygen-containing groups elicits an opening of band gap in graphene. In this work, we aim to induce an optical response in graphene via controlled oxidation, and then explore potential origins of its photoluminescence through mathematical modeling. We employ timed ozone treatment of initially non-fluorescent reduced graphene oxide (RGO) to produce graphene oxide (GO) with specific optical properties. Oxidized material exhibits substantial changes in the absorption spectra and a broad photoluminescence feature, centered at 532 nm, which suggests the appearance of a band gap. We then explore a number of possible mechanisms for the origin of GO photoluminescence via PM3 and ab initio calculations on a functionalized single sheet of graphene. By adjusting modeling parameters to fit experimentally obtained optical transition energies we estimate the size of the sp^2 graphitic regions in GO and the arrangement of functional groups that could be responsible for the observed emission.

Nicholas Lombardo
Central Conencticut State University

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