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Infrared Spectroscopy of Functionalized Graphene Sheets from First Principle Calculations CUI ZHANG, Department of Chemistry, Princeton University, DANIEL DABBS, ILHAN AKSAY, Department of Chemical and Biological Engineering, Princeton University, ROBERTO CAR, ANNABELLA SELLONI, Department of Chemistry, Princeton University — Detailed characterization of the structure of functionalized graphene sheets (FGSs) is an important and challenging task which could help to improve the performance of FGS materials for technological applications. We present here first principles calculations for the infrared (IR) spectra of different FGS models aimed at identifying the IR signatures of different functional groups and defect sites on FGSs. We found that vacancies and edges have significant effects on the IR frequencies of the functional groups on FGSs. In particular, hydroxyl groups close to vacancies have higher stretching and lower bending frequencies in comparison to hydroxyls in defect free regions of FGSs. More interestingly, the OH vibrations of carboxyl groups at edges exhibit unique features in the high frequency IR bands, which originate from the interactions with neighboring groups and the relative orientation of the carboxyl with respect to the FGS plane. Our results are supported by experimental IR measurements on FGS powders.

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