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Chemical functionalization of suspended graphene membrane - a combined first-principles and experimental study WEI WANG, EFTHIMIOS KAXIRAS, ROBERT WESTERVELT, Harvard University — A single-atomic layer membrane, graphene is a unique material with ultimate large surface area for a given volume. These surfaces are inert and stable enough to confront rather harsh chemical and/or physical environment and maintains its structural integrity, yet they are active and versatile enough to chemically interact with various absorbate and form new crystalline or disordered structures that trigger dramatic change of its properties such as conductor-isolator transition. In this study, we use first principle calculations to explore the interactions among graphene and a variety of ions and functional groups, showing how each of these species or the combination of these species interact with graphene and in turn change its structural, electric, magnetic and phonon properties. In addition, we discuss experimentally detecting and characterizing chemically functionalized graphene structure with Raman spectroscopy and aberration corrected transmission electron microscopy.

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