First-Principles DFT Studies of the Vibrational Properties of Germanene Nanoflakes

STEVEN RICHARDSON, Department of Chemistry, Massachusetts Institute of Technology and Department of Electrical Engineering and Computer Science, Howard University, BORJA PEROPARDE, XAVIER ANDRADE, ALN ASPURU-GUZIK, Department of Chemistry and Chemical Biology, Harvard University — The germanium analogue of graphene, germanene, is a potentially new atomically thin quantum material which theory predicts will possess unique transport and optoelectronic properties. Recently, there have been a number of experimental efforts to successfully grow two-dimensional films of germanene on noble metal substrates using molecular beam epitaxy. In addition to this top-down approach of synthesizing large scale films of germanene, we would like to focus on a bottom-up approach where nanoflakes of germanene could be used as molecular seeds or precursors to grow large films of two-dimensional germanene. A knowledge of their infrared and Raman spectra will be critical for characterizing these germanene nanoflakes in future experiments. In this work we used density-functional theory (DFT) to compute the vibrational spectra of a selected number of lower order germanene nanoflakes (e.g. hexagermabenzenene, germa-naphthalene, germa-anthracene, germa-phenanthrene, germa-pyrene, germa-tetracene, and germa-pentacene). Our DFT studies also reveal that these germanene nanoflakes are vibrationally stable with buckling of these molecules from their normal two-dimensional planar forms which exist in graphene nanoflakes.

This research is supported by NSF Grant No. DMR-1231319

Steven Richardson
Massachusetts Institute of Technology; Howard University