Abstract Submitted
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First-Principles DFT Studies of the Vibrational Properties of Germanene Nanoflakes[1] 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. hexagermabenzene, *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.

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