Novel Quantum Materials Beyond Graphene: Germanene Nanoflakes

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While graphene has remarkable transport properties, it does not possess a band gap and thus has limited applications in device physics. It is therefore important to both identify and study new two-dimensional atomically thin quantum materials beyond graphene. Germanene, the germanium analog of graphene, is one such example of a new quantum material. The large spin-orbit coupling present in germanium alters its electronic structure to produce novel transport and optoelectronic properties than are not seen in graphene.

Recently, there has been some progress in the synthesis of thin films of germanene and germanane, the hydrogenated form of germanene, using both top-down processes like molecular beam epitaxy and chemical vapor phase deposition and a bottom-up process such as direct chemical synthesis. We would like to suggest an additional approach to the bottom-up process by using germanium nanoflakes to serve as molecular seeds or precursors for the large-scale growth of pure sheets of germanene in chemical vapor phase deposition experiments.

To help guide future experimental work in how germanene nanoflakes might be used to grow large-scale films of germanene, we have used density-functional theory to calculate the electronic, structural, vibrational, and optical properties of several lower-order germanene nanoflakes such as hexagermabenzene (Ge_6H_6), *germa*-naphthalene ($Ge_{10}H_8$), *germa*-anthracene ($Ge_{14}H_{10}$), *germa*-phenanthrene ($Ge_{14}H_{10}$), and *germa*-pyrene ($Ge_{16}H_{10}$). We have determined that these nanoflakes are thermodynamically stable with a geometry that is buckled due to pseudo-Jahn Teller distortions from the planar forms that are present in graphene nanoflakes. In addition, we have computed accurate infrared and Raman spectra for a family of selected germanene nanoflakes. Our first-principles studies on the properties of germanene nanoflakes will be critical for characterizing these molecules in future experimental efforts.