Electronic Supplementary Information

Phonon vortices at heavy impurities in two-dimensional materials

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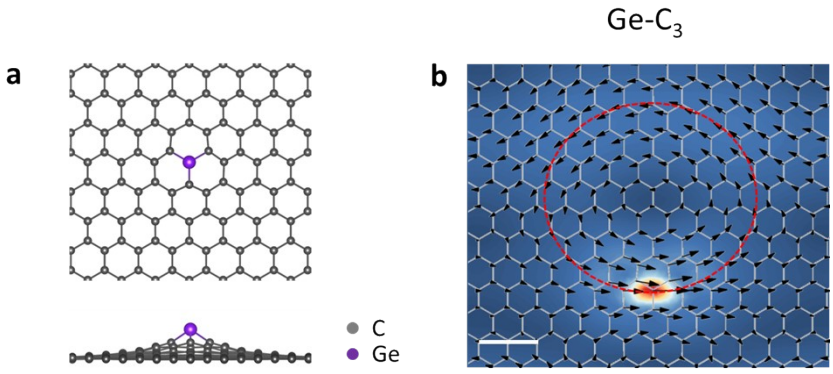

Figure S1. Phonon vortex in Ge-C_3 -- one C atom is replaced by one Ge atom, *i.e.*, an impurity atom that is larger and heavier than Si. Calculations were performed in a 12×12 supercell as in Figure 1d for Si-C_3 because of the computational cost, but the presence of a vortex is clear.

a) In-plane and side view schematics of the Ge-C_3 defect showing that the Ge atom buckles by 2.2 Å off the graphene plane, compared with the 1.8-Å buckling by Si in Si-C_3. b) Atomic displacements around a Ge-C_3 defect at $\hbar w$ = 26 meV showing clearly that Ge generates a larger vortex than Si, as illustrated by the red circle that goes through the Ge site which is much larger than the corresponding red circle of the Si-C_3-defect vortex in Fig. 1d. Another notable feature is that the atomic displacements of C atoms forming circles that are concentric with the red circle are pointing in the same direction, in contrast to the Si-C_3 defect, where the atomic displacements in the two red circles shown in Fig. 1 are in opposite directions. This feature is most likely related to the fact that the wavelength of the pristine-graphene mode that is in resonance with the Ge-C_3 vortex mode is much longer than in the case of the Si-C_3 vortex mode. Much larger computational supercells, perhaps even larger than 24×24 would be needed to explore these issues further with sufficient accuracy. Scale bar: 0.5 nm.