

Supplementary information:

Stability and electronic properties of gallenene

Alex Kutana,^a Tariq Altalhi,^b Qiyuan Ruan,^a Jun-Jie Zhang,^a Evgeni S. Penev,^a
and Boris I. Yakobson^{*,b,c}

*a Department of Materials Science and NanoEngineering, Rice University, Houston, Texas
77005, United States*

b Chemistry Department, Taif University, Taif 21974, Saudi Arabia

c Department of Chemistry, Rice University, Houston, Texas 77005, United States

E-mail: biy@rice.edu

Interaction potential for gallene on unreconstructed Si(111) substrate

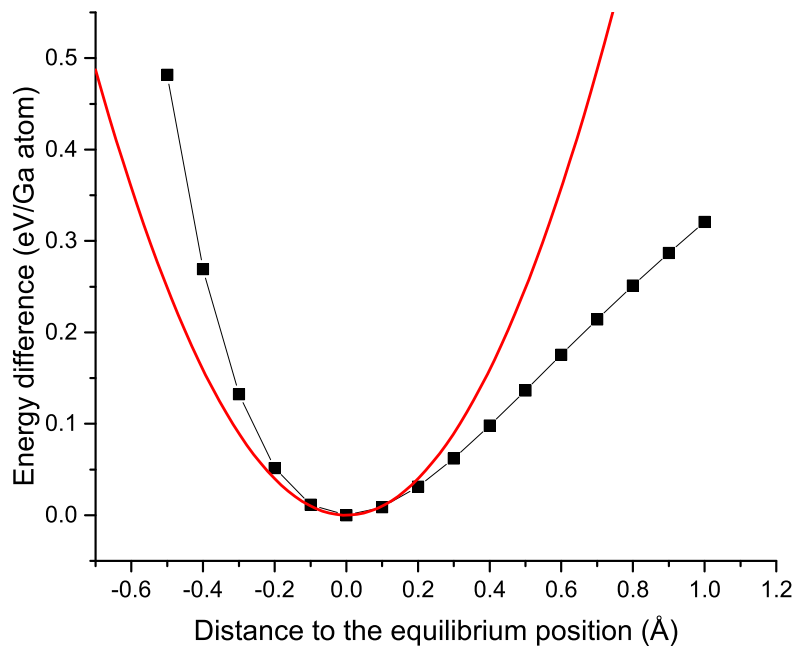


Figure S1: Interaction potential for gallene on unreconstructed Si(111) substrate calculated with DFT.

Parameters for T_c calculations in gallene

structure	k -mesh	q -mesh	ω_{ln} (K)	λ	T_c (K)
14₂	28×20	28×20	63.4	1.51	7.3
40	32×32	16×16	91.5	1.07	7.1
10	21×21	7×7	82.3	0.91	4.9
27	24×16	12×8	86.6	1.14	7.3

Band structure of gallenene

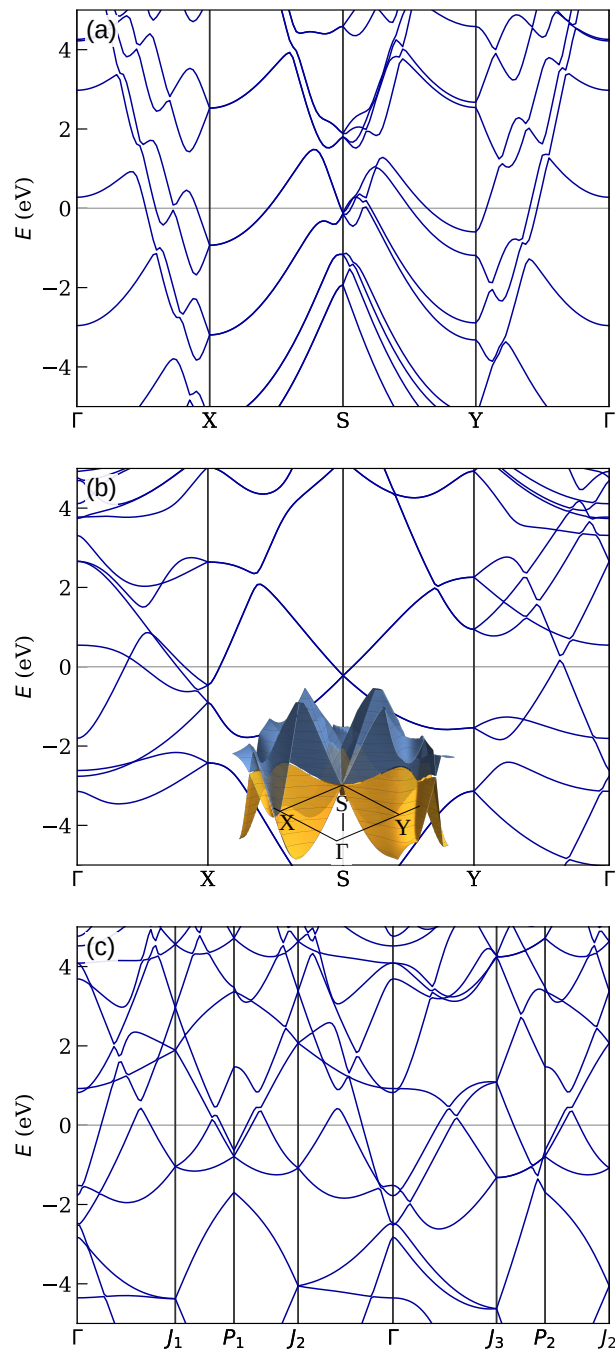


Figure S2: Electronic band structures of gallenene structures (a) **40**, (b) **14₁**, and (c) **14₂**. The inset in (b) shows the two bands that cross at the S point (rendered in the energy window $E_F \pm 2$ eV and only over 3/4 of the Brillouin zone for clarity), indicating presence of a nodal line near the Fermi level.

Electronic density of states

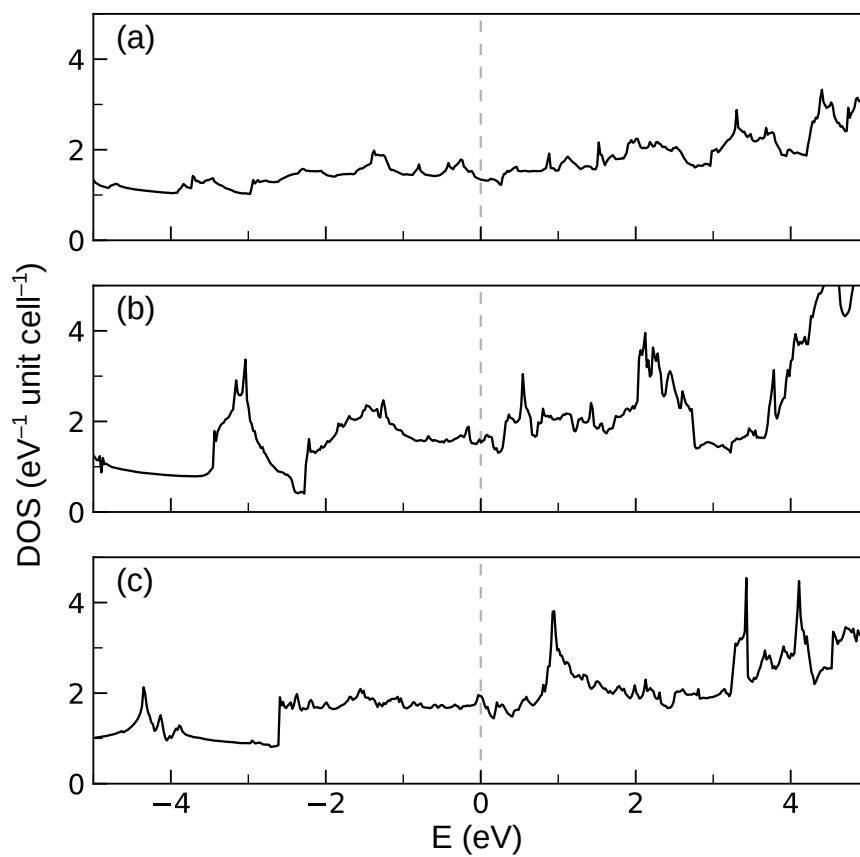


Figure S3: Electronic densities of states of gallene structures (a) **40**, (b) **14₁**, and (c) **14₂**.

Gallenene structures 12 and 23

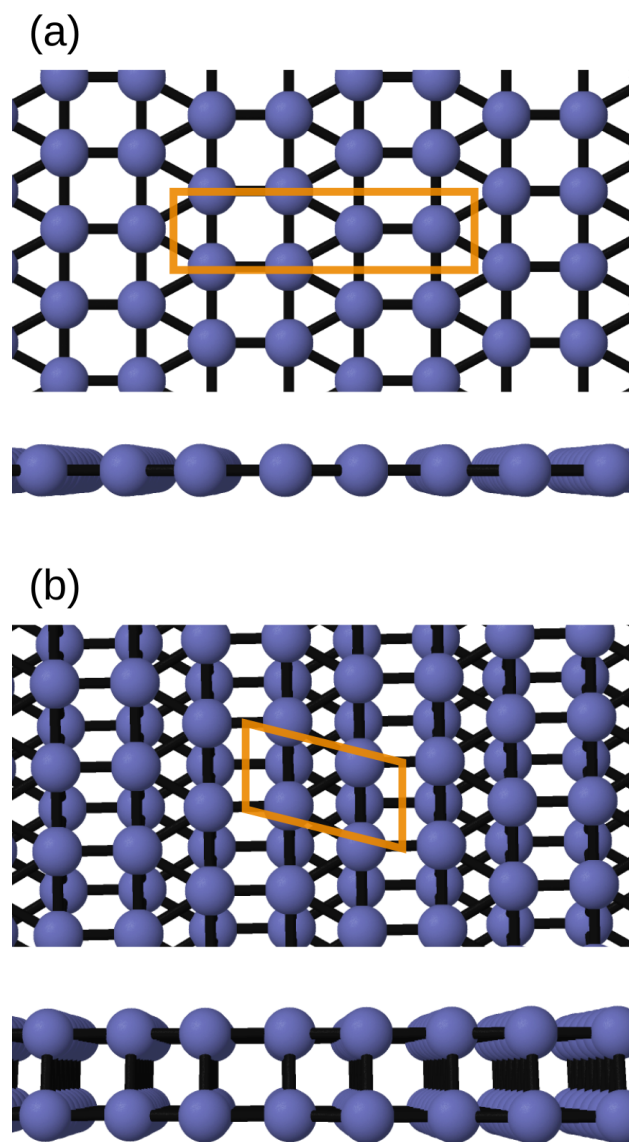


Figure S4: Gallenene structures (a) **12** and (b) **23**.

Visualizations of unstable out-of-plane and in-plane phonon modes

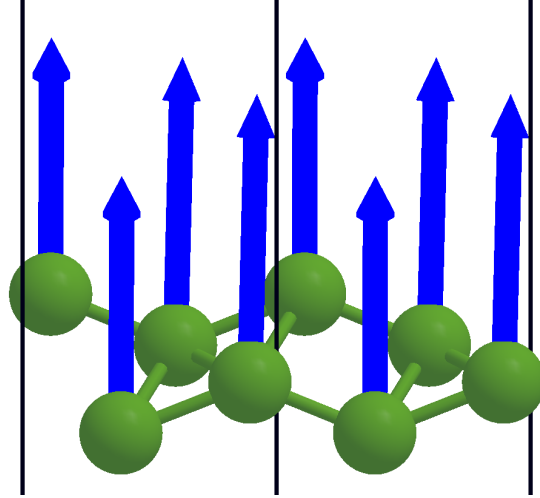


Figure S5: Visualization of the unstable out-of-plane phonon mode along Γ -X direction in Figure 3b of the main text.

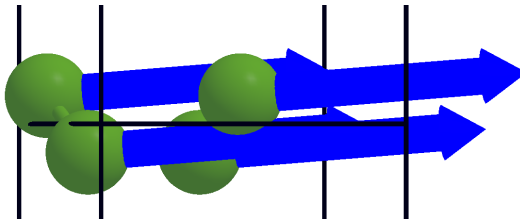


Figure S6: Visualization of the unstable in-plane phonon mode along Γ -J₁ direction in Figure 4b of the main text.