Electrons and phonons in 2D materials

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Recently, several carbon allotropes with sp^2 and sp^3 hybridization were predicted theoretically and some are candidates to show Dirac's cones [1-3]. Here we study the electron and phonon properties of one of these new allotropes of two-dimensional carbon called phagraphene, consisting of rings with 5, 6 and 7 atoms (Figure 1a) [4]. This stable structure is energetically relatively close to graphene compared to other allotropes of carbon due to its sp^2 hybridization and dense atomic packing. The existence of a Dirac cone distorted in the first Brillouin zone of this structure was shown by both density functional theory (DFT) and tight-binding calculations [4].

Our investigations are based on DFT as implemented in SIESTA [5]. Electron and phonon band structures (Figure 1b,c) and density of states are computed with a finite difference scheme using Inelastica [6]. With TranSIESTA [7] we further explore electronic transport through interfaces between phagraphene and graphene (Figure 1d).

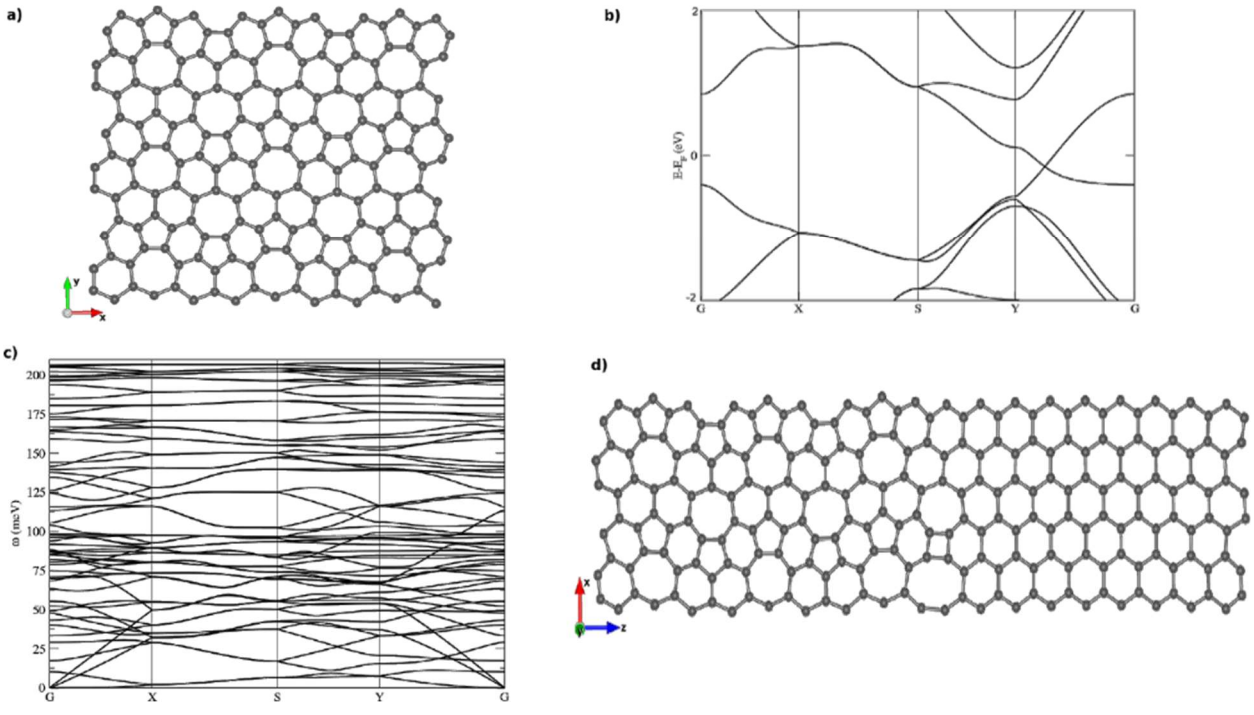

Figure 1: a) Phagraphene structure in a 3×3 repetition of the 20-atom unit cell, b) Electron band structure revealing a Dirac cone at the Fermi energy, c) Phonon band structure, d) Example of an interface structure between phagraphene and graphene for transport studies.

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