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Athos-graphene: a metallic carbon allotrope

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Abstract:

Metallic two-dimensional carbon allotropes are attractive lithium-ion battery anodes, but many predicted structures are semiconducting or show high Li diffusion barriers [1]. We investigate Athos-graphene (AG), a planar sp2 carbon monolayer built from the dicyclobuta[de,ij]naphthalene motif, inspired by the tile mosaics of Brazilian artist Athos Bulcão. The orthorhombic lattice has 12 atoms per unit cell, combining four-, five-, and twelve-membered rings in a porous network. We used density functional theory with the PBE functional at SIESTA/TRANSISESTA code [2]. Direction-dependent conduction has been reported for nanoribbons of the non-hexagonal allotrope OPG-Z [3], and AG is likewise anisotropic: its Young's modulus peaks at 325 N/m along x and drops markedly along other directions, and its optical absorption depends on the polarization direction. AG is metallic, with two bands crossing the Fermi level. Double-sided Li adsorption is favorable at all coverages, with energies from −2.39 to −0.9 eV. Lithiation with 18 Li atoms per supercell gives a theoretical capacity of 836.78 mAh/g, above graphite (372 mAh/g) and graphene (744 mAh/g), and an average open-circuit voltage of 0.54 V that stays positive during lithiation. The lowest in-plane diffusion barrier is 0.30 eV across five-membered rings, slightly below the 0.32 eV of graphene [4], with diffusion coefficients above 10−6 cm2/s at room temperature. Diffusion across the twelve-membered rings is hindered (1.04 to 1.42 eV) and interlayer migration needs 0.66 eV. These results identify AG as a stable, metallic anode candidate with high capacity for electronic transport.

References:

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