Exotic Band Topologies in Carbon Allotropes

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Carbon is one of the most fundamental elements in nature hosting tremendous allotropes benefitting from its ability to form *sp*, sp^2, and sp^3 hybridized carbon-carbon bonds. The search of new carbon allotropes is always in the spotlight of condensed matter physics and materials sciecnes. Besides the experimental efforts, the predictions and investigations for carbon structures based on *ab initio* calculations is also an active research field. In recent years, topological materials have been attracting tremendous research interests and a series of carbon allotropes are reported to hold exoric band topologies, especially topological nodal lines. In this work, we report a series of carbon allotropes[1-4] as topological nodal line semimetals including: (i) sp^2-sp^3 hybridized oP16 carbon[1] hosting two closed nodal rings in the k_y=0 and k_y=π mirror planes, and oP16 carbon is the first reported sp^2-sp^3 hybridized carbon structure with closed nodal rings; (ii) all-sp^2 hybridized bct-4 carbon[2] with a large nodal ring in the k_z=0 mirror plane, previously bct-4 carbon has long been thought as a simple metallic carbon, actually it is a nodal line semimetal with a large closed nodal ring; (iii) hybrid nodal chain in all-sp^2 hybridized oP-C_{24} carbon[3], oP-C_{24} carbon has a closed nodal ring in the k_y=0 mirror plane and four antenna-like nodal lines connecting with the nodal ring forming a chain network, which are protected with only spatial inversion, time reversal and mirror symmetries and can be explained based on a two-band effective model; (iv) nodal rings in sp^2-sp^3 hybridized polymerized carbon nanotubes CNT(5,0) and CNT(7,0) carbon[4], CNT(5,0) and CNT(7,0) has the same space group symmetries but distinct electronic properties, we provide an explanation for this phenomenon from the real space crystalline perspective.

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References

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