Tight-binding theory of spin-orbit coupling in graphynes

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Outline

- Graphynes
- Tight-binding theory
- Spin-orbit coupling
- Results
- Conclusion
Graphynes

- 2D carbon allotropes

Graphynes

- Dirac-like bandstructures and gapped systems
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- Dirac-like bandstructures and gapped systems

Focus: Graphyne May Be Better than Graphene

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Sheets of single-layer carbon with a variety of bonding patterns may have properties similar to the wonder material graphene, according to new computer simulations.

Super-strong, highly conducting graphene is the hottest ticket in physics, but new computer simulations suggest that materials called graphynes could be just as impressive. Graphynes are one-atom-thick sheets of carbon that resemble graphene, except in the type of atomic bonds. Only small pieces of graphyne have so far been fabricated, but the new simulations, described in Physical Review Letters, may inspire fresh efforts to construct larger samples. The authors show that three different graphynes have a graphenelike electronic structure, which results in effectively massless electrons. The unique symmetry in one of these graphynes may potentially lead to new uses in electronic devices, beyond those of graphene.

Graphynes

- Graphdiyne has been synthesized

β-graphyne

- 18 atoms in the unit-cell
- 3 different hopping parameters
- 6 Dirac cones

\[ t_{\beta,1} = -2.00 \text{eV} \]
\[ t_{\beta,2} = -2.70 \text{eV} \]
\[ t_{\beta,3} = -4.30 \text{eV} \]
β-graphyne

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Spin-orbit coupling

- Intrinsic SOC results from relativistic corrections to the Schrödinger equation, that couples the spin and orbital angular momentum

\[ H_L = -\frac{\hbar}{4mc^2} \sigma \cdot (p \times \nabla V) = -f(r)\sigma \cdot L \]

- Rashba SOC results from broken mirror symmetry in z direction, due to an external electric field

\[ H_E = Ez \]
Spin-orbit coupling

Intrinsic SOC results from relativistic corrections to the Schrödinger equation, that couples the spin and orbital angular momentum.

Rashba SOC results from broken mirror symmetry in the z direction, due to an external electric field.
SOC and tight-binding theory

- SOC-free TB model: $p_z$ & $\{s, p_x, p_y\}$-orbitals, decouple by reflection symmetry and absence of spin

- Intrinsic SOC couples $p_z, \uparrow(\downarrow)$ to $p_x, \downarrow(\uparrow)$ and $p_y, \downarrow(\uparrow)

\[
\begin{array}{c|c|c|c}
\sigma \cdot L & p_x & p_y & s \\
p_z & -i\sigma_y & i\sigma_x & 0 \\
\end{array}
\]

- Rashba SOC couples $p_z, \uparrow(\downarrow)$ to $s, \uparrow(\downarrow)$
SOC and tight-binding theory

\( p_z \)-orbitals

\( s, p_x, p_y \)-orbitals
SOC and tight-binding theory

- Since SOC couples the $p_z$ orbitals to $\sigma$-orbitals

\[
H = H_z + H_\sigma
\]

Due to SOC

\[
H = H_z + H_\sigma + H_{\text{SOC}}^{z,\sigma} + (H_{\text{SOC}}^{z,\sigma})^\dagger
\]

- Apply low-energy approximation to eliminate $\sigma$-orbitals

\[
H_{z,v+e}^{\text{eff}} = H_z - H_{\text{SOC}}^{z,\sigma} H_\sigma^{-1} (H_{\text{SOC}}^{z,\sigma})^\dagger
\]
SOC Hamiltonian for effective model

- For $\beta$-graphyne this yields

\[
H_{R,\beta} = i\lambda_{\text{int},R} \sum_{\langle i,j \rangle} \dot{p}^\dagger_{z,i} \left( \sigma \times \hat{d}_{ij} \right) \cdot \hat{z} p_{z,j} + i\lambda_{\text{ext},R} \sum_{\langle i,j \rangle} \ddot{p}^\dagger_{z,i} \left( \sigma \times \hat{d}_{ij} \right) \cdot \hat{z} p_{z,j}
\]

\[
H_{I,\beta} = i\lambda_{\text{int},I} \sum_{\langle\langle i,j \rangle\rangle} \dot{v}_{ij} p^\dagger_{z,i} \sigma_{z} p_{z,j} + i\lambda_{\text{ext},I} \sum_{\langle\langle i,j \rangle\rangle} \ddot{v}_{ij} p^\dagger_{z,i} \sigma_{z} p_{z,j}
\]
Rashba SOC in \( \beta \)-graphyne

Increasing **internal** Rashba

Increasing **external** Rashba

\[
\frac{t_{\text{ext}}}{t_{\text{int}}} = -1.18.
\]

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Rashba SOC in $\beta/\gamma$-graphyne

Intrinsic SOC in $\beta$-graphyne

- Trivial or topological gap?

- Corresponds to QSHE

\[ \frac{t_{\text{ext}}}{t_{\text{int}}} = -1.18 \]
Conclusions

- Very general method to address SOC in planar carbon structures
- External and internal SOC
- In $\beta(\gamma)$-graphyne the internal (external) Rashba can open (close) a gap
- $\beta$-graphyne exhibits high-Chern number bands under influence of intrinsic SOC

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