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

R. H. Baughman, H. Eckhardt, and M. Kertesz, J. Chem. Phys. 87, 6687 (1987)
Graphynes

- Dirac-like bandstructures and gapped systems
Graphynes

- Dirac-like bandstructures and gapped systems

Malko, Neiss, Viñes, and Görling, PRL 108, 086804 (2012)
Graphynes

Graphdiyne has been synthesized

G. X. Li, Y. L. Li, H. B. Liu, Y. B. Guo, Y. J. Li and D. B. Zhu, Chem. Commun., 2010, 46, 3256–3258.
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**

- 18 atoms in the unit-cell
- 3 different hopping parameters
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\[
\begin{align*}
t_{\beta,1} &= -2.00\text{eV} \\
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\end{align*}
\]
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 z direction, due to an external electric field.

Two-dimensional carbon topological insulators superior to graphene

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Graphene was the first material predicted to realize a topological insulator (TI), but unfortunately the gap is unobservably small due to carbon’s weak spin-orbital coupling (SOC). Based on first-principles calculations, we propose a stable sp-sp\(^2\) hybrid carbon network as a graphene analog whose electronic band structures in proximity of the Fermi level are characterized by Dirac cones. We demonstrate that this unique carbon framework has topologically nontrivial electronic structures with the \(Z_2\) topological invariant of \(v=1\) which is quite promising for hosting the quantum spin Hall effect (QSHE) in an experimentally accessible low temperature regime (<7 K). This provides a viable approach for searching for new TIs in 2D carbon allotropes.
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 $p_y, \downarrow(\uparrow)$

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

- 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

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

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

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

- For $\beta$-graphyne this yields

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

\[
H_{I,\beta} = i\lambda_{\text{int},I} \sum_{\langle\langle i,j \rangle\rangle} \dot{v}_{ij} \dot{p}_{z,i}^\dagger \sigma_z \dot{p}_{z,j} + i\lambda_{\text{ext},I} \sum_{\langle\langle i,j \rangle\rangle} \dot{v}_{ij} \dot{p}_{z,i}^\dagger \sigma_z \dot{p}_{z,j}
\]
Rashba SOC in $\beta$-graphyne

Increasing \textcolor{red}{\textit{internal}} Rashba

Increasing \textcolor{blue}{\textit{external}} Rashba

$\frac{t_{\text{ext}}}{t_{\text{int}}} = -1.18$
Rashba SOC in $\beta/\gamma$-graphyne

GvM, V. Juričić, and C. Morais Smith arXiv:1409.0388
Intrinsic SOC in $\beta$-graphyne

- Trivial or topological gap?

$$t_{\text{ext}}/t_{\text{int}} = -1.18.$$  

- Corresponds to QSHE
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

GvM, V. Juričić, and C. Morais Smith arXiv:1409.0388
GvM, C. Morais Smith, and V. Juričić PRB 90, 081406(R)