Tight-binding theory of spin-orbit coupling in graphynes

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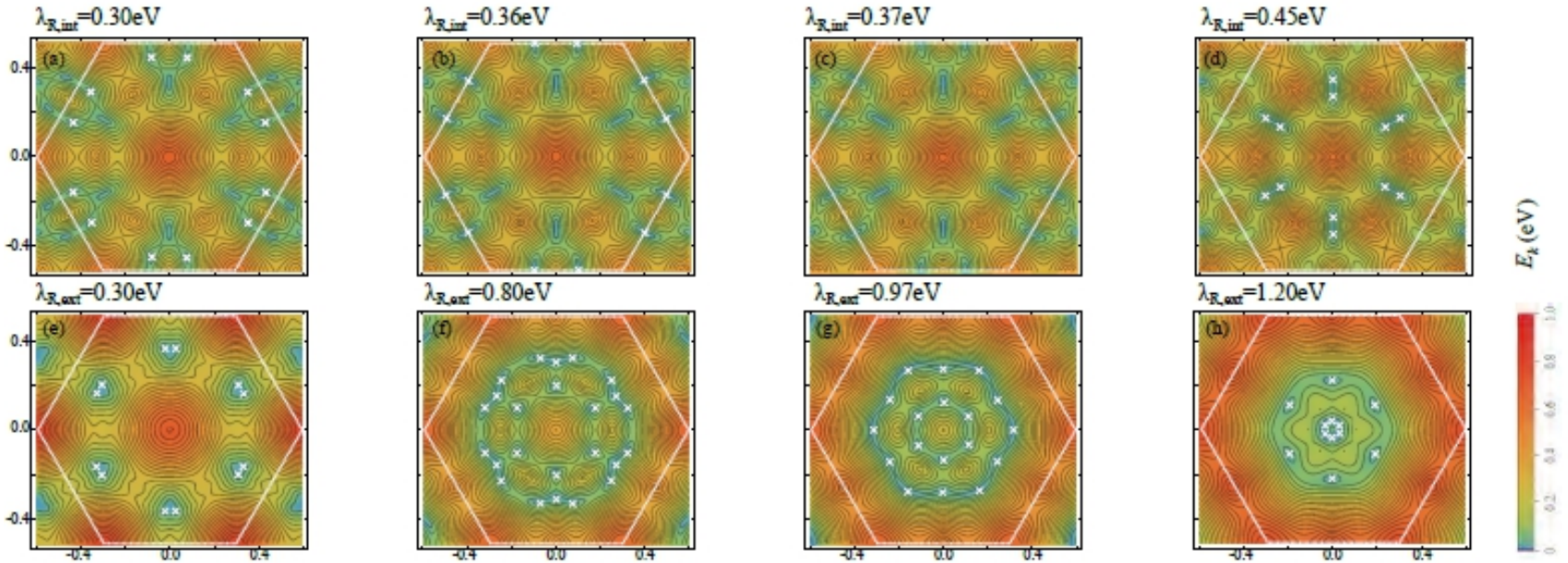


Collaborators:
Cristiane Morais Smith & Vladimir Juričić

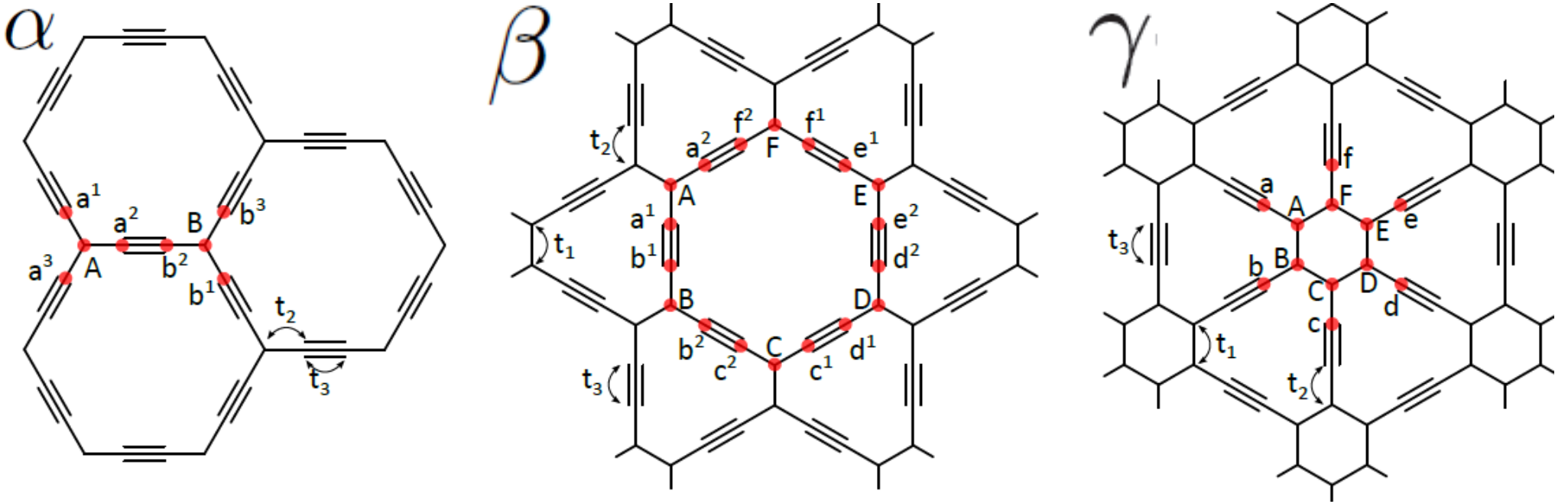
Outline

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

Graphynes

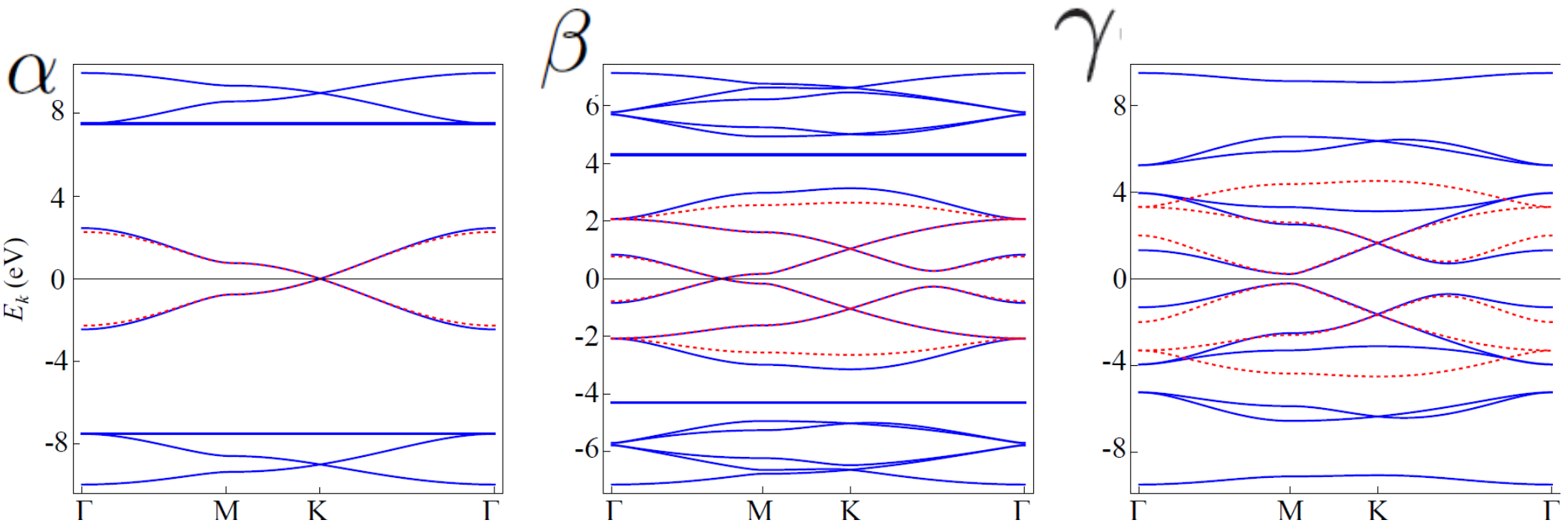
- 2D carbon allotropes

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

Focus: Graphyne May Be Better than Graphene

Published February 24, 2012 | Physics **5**, 24 (2012) | DOI: 10.1103/Physics.5.24

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.

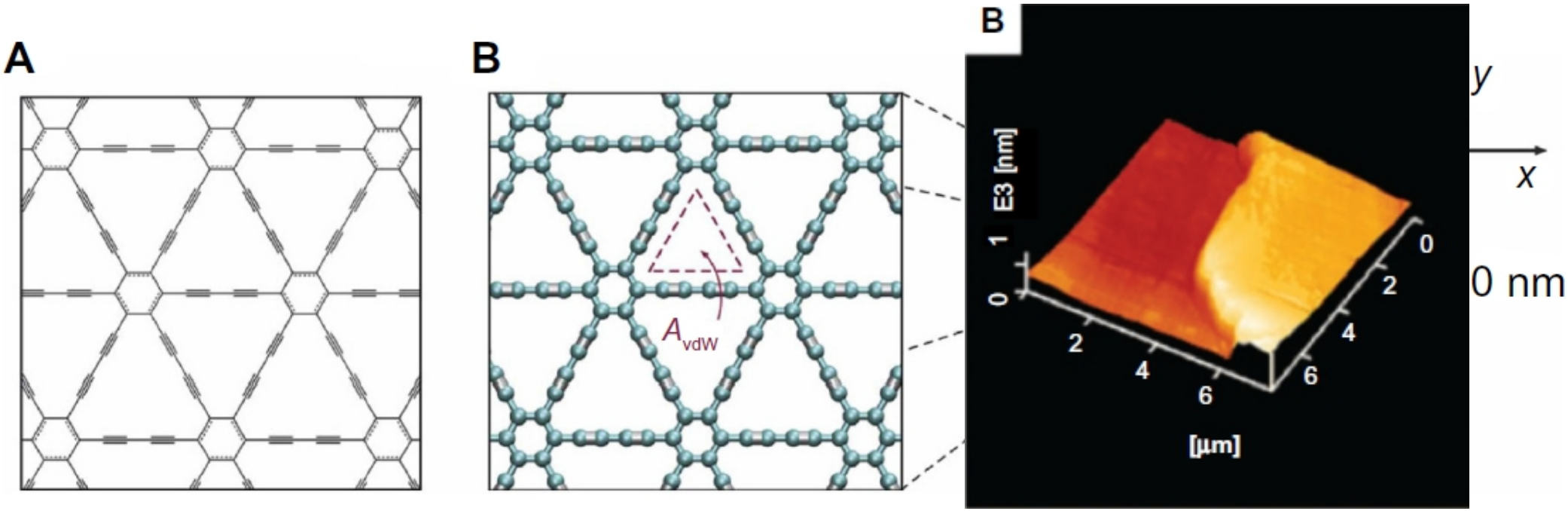
Competition for Graphene: Graphynes with Direction-Dependent Dirac Cones
Daniel Malko, Christian Neiss, Francesc Viñes, and Andreas Görling
Phys. Rev. Lett. **108**, 086804 (2012)
Published February 24, 2012

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

Graphynes

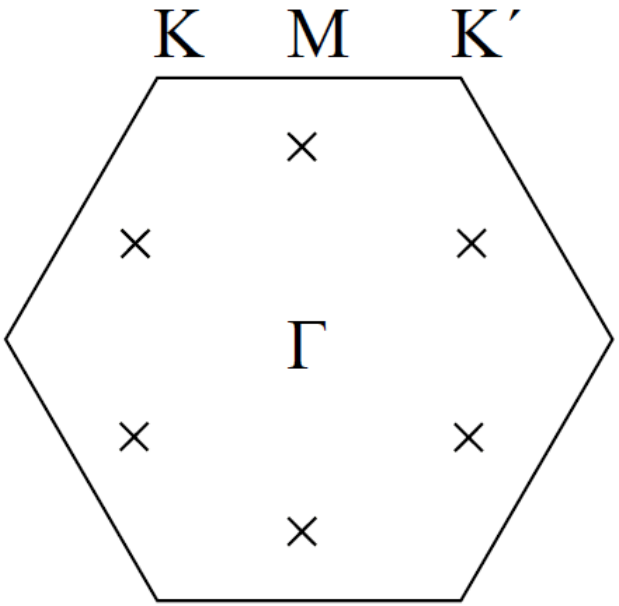
- Graphdiyne has been synthesized

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.

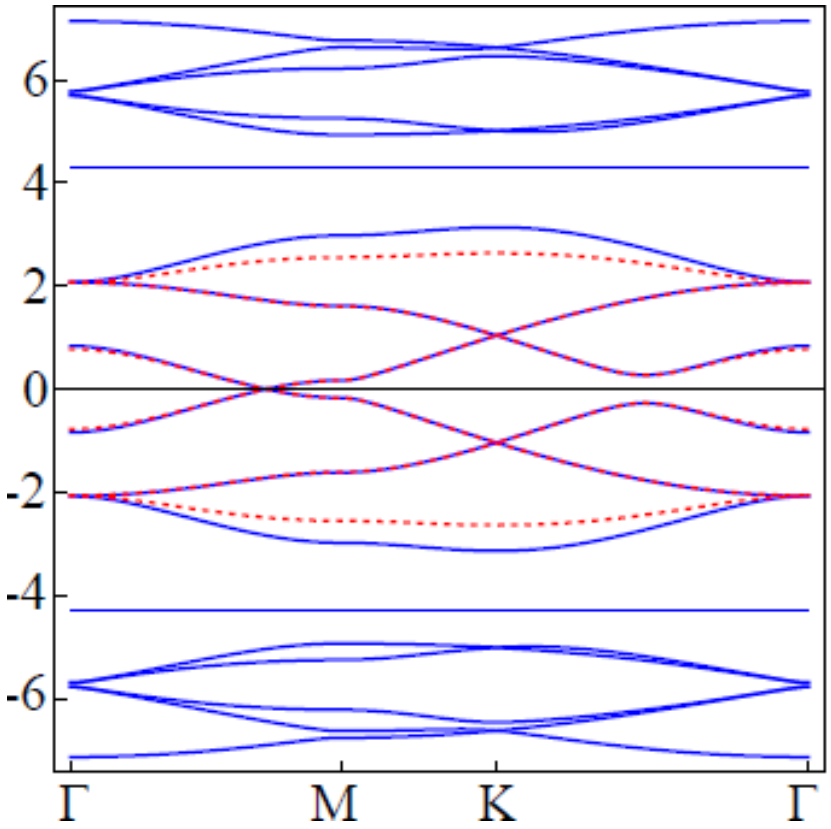


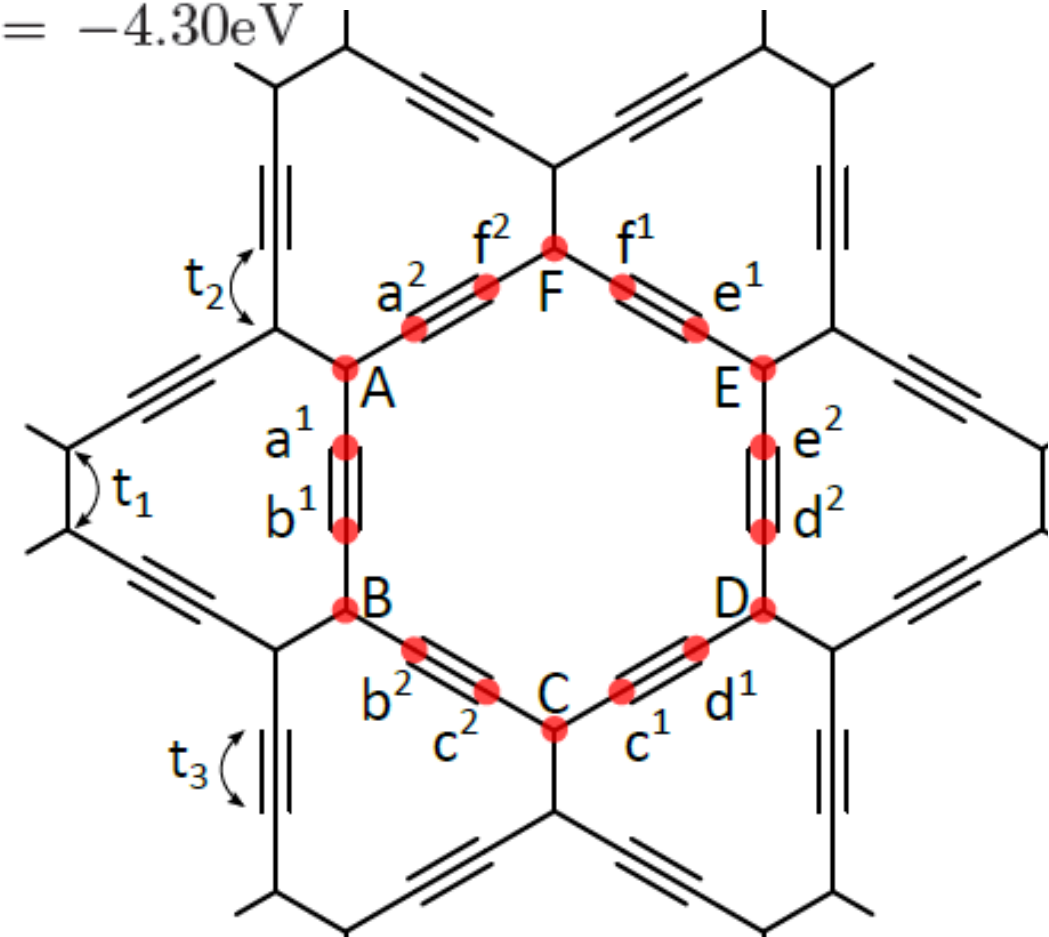
β-graphyne

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



$$t_{\beta,1} = -2.00\text{eV}$$
$$t_{\beta,2} = -2.70\text{eV}$$
$$t_{\beta,3} = -4.30\text{eV}$$





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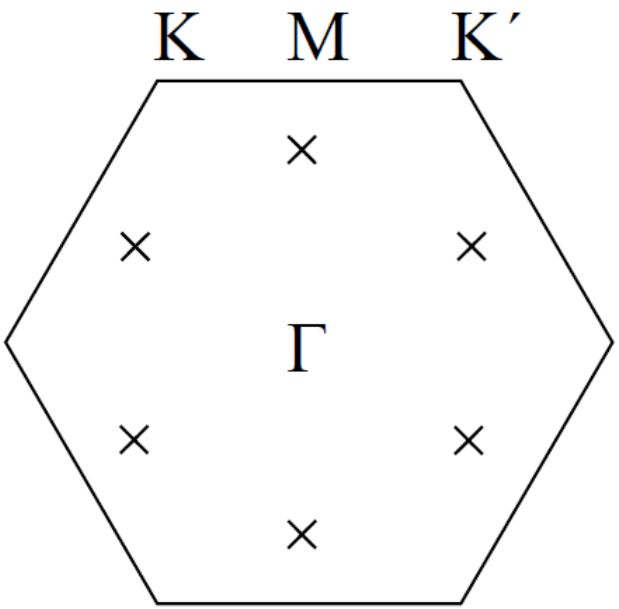

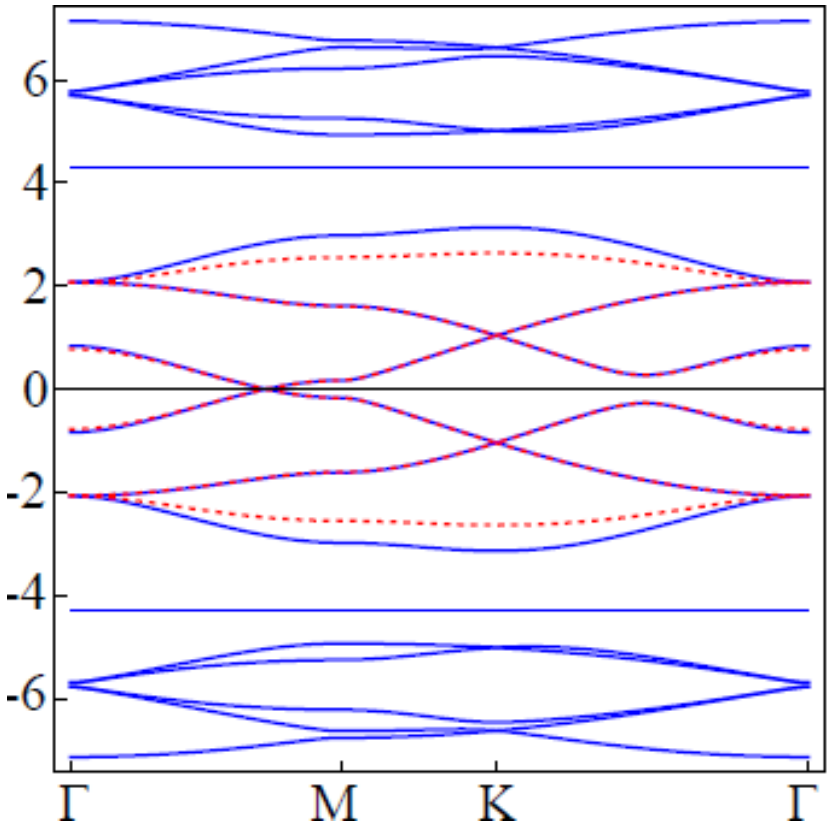

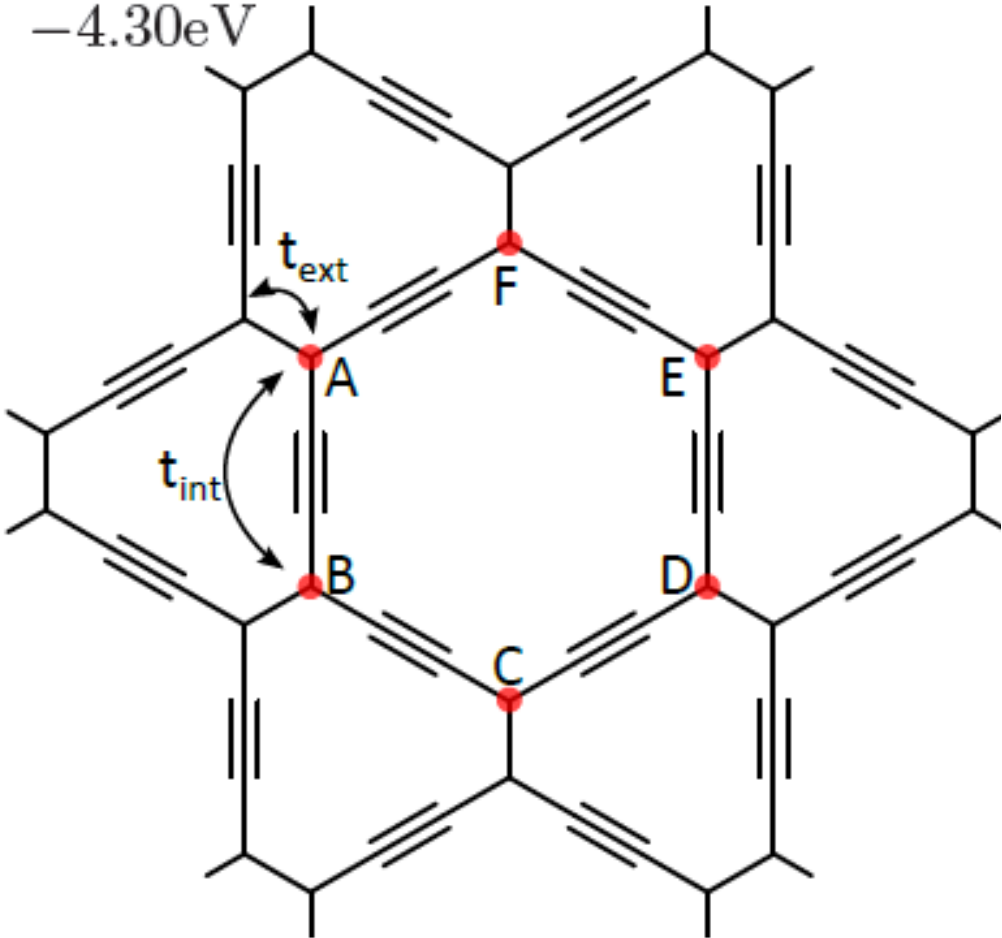

Spin-orbit coupling

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

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

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

$$H_E = Ez$$

Spin-orbit coupling

SCIENTIFIC REPORTS

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SUBJECT AREAS:

TOPOLOGICAL INSULATORS

TWO-DIMENSIONAL MATERIALS

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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 $p_{y,\downarrow(\uparrow)}$

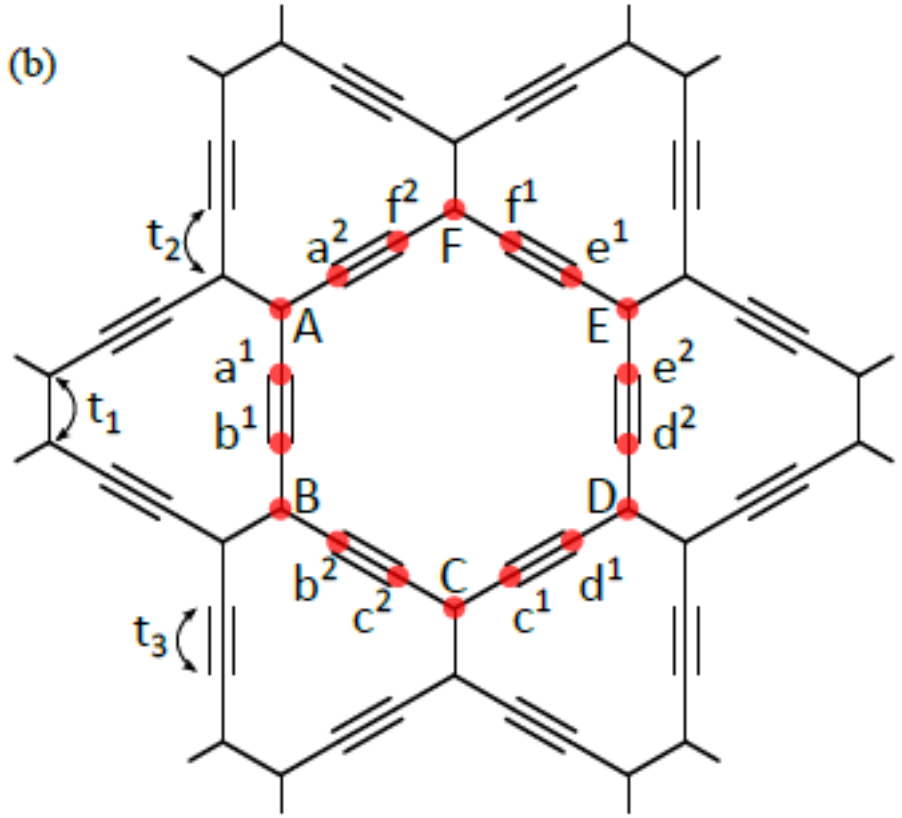
$\boldsymbol{\sigma}\cdot\boldsymbol{L}$	p_x	p_y	s
p_z	$-i\sigma_y$	$i\sigma_x$	0

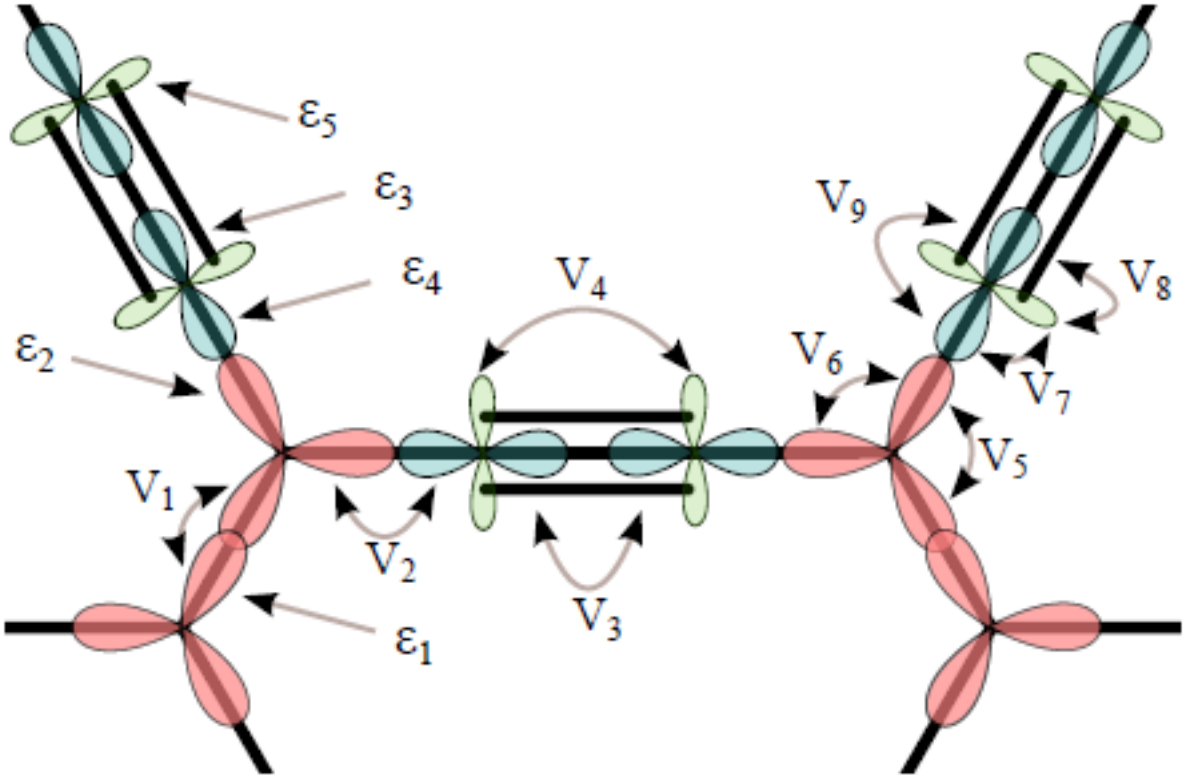
- Rashba SOC couples $p_{z,\uparrow(\downarrow)}$ to $s_{\uparrow(\downarrow)}$

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 σ-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 σ-orbitals

$$H_{z,v+e}^{\text{eff}} = H_z - H_{SOC}^{z,\sigma} H_\sigma^{-1} (H_{SOC}^{z,\sigma})^\dagger$$

SOC Hamiltonian for effective model

- For β-graphyne this yields

$$H_{R,\beta} = i\lambda_{\mathrm{int,R}} \sum_{\langle i,j \rangle}^{\cdot} p_{z,i}^{\dagger} \left(\boldsymbol{\sigma} \times \hat{\mathbf{d}}_{ij} \right) \cdot \hat{\mathbf{z}} p_{z,j} + i\lambda_{\mathrm{ext,R}} \sum_{\langle i,j \rangle}^{\cdot\cdot} p_{z,i}^{\dagger} \left(\boldsymbol{\sigma} \times \hat{\mathbf{d}}_{ij} \right) \cdot \hat{\mathbf{z}} p_{z,j}$$

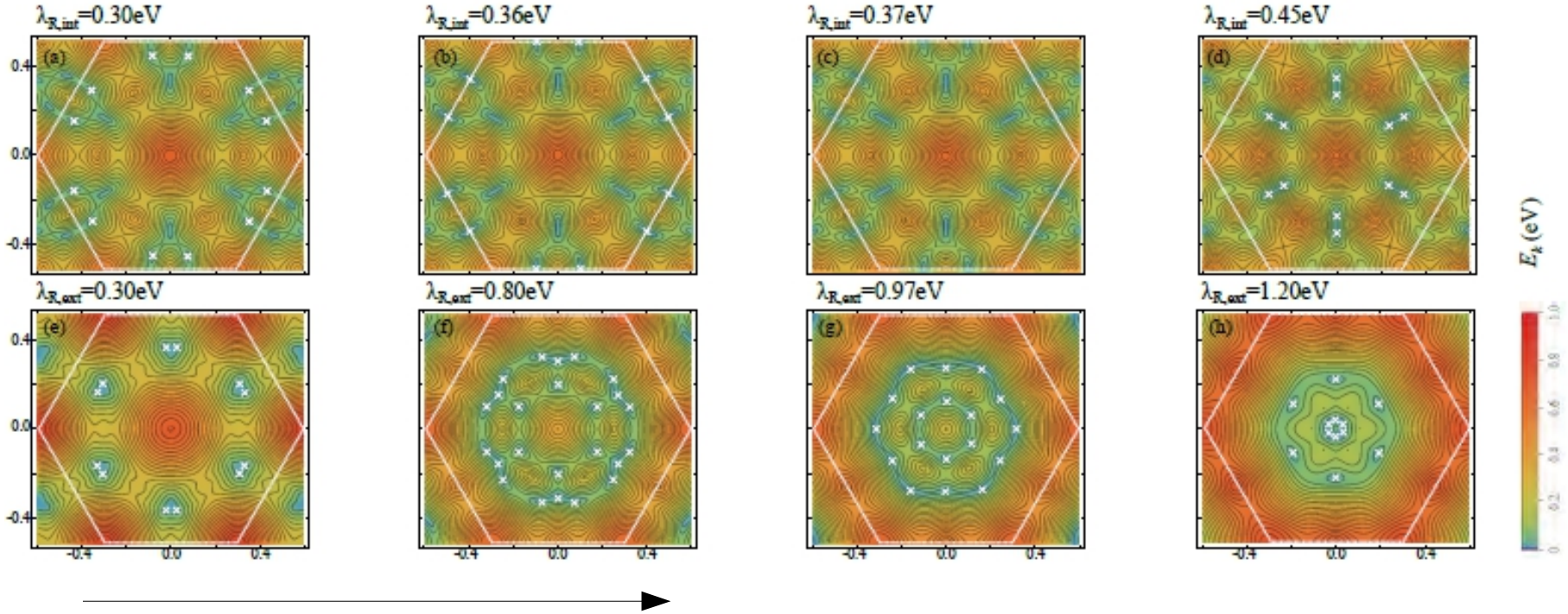
$$H_{I,\beta} = i\lambda_{\mathrm{int,I}} \sum_{\langle\langle i,j \rangle\rangle}^{\cdot} v_{ij} p_{z,i}^{\dagger} \sigma_z p_{z,j} + i\lambda_{\mathrm{ext,I}} \sum_{\langle\langle i,j \rangle\rangle}^{\cdot\cdot} v_{ij} p_{z,i}^{\dagger} \sigma_z p_{z,j}$$

Rashba SOC in β-graphyne

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

Increasing internal Rashba

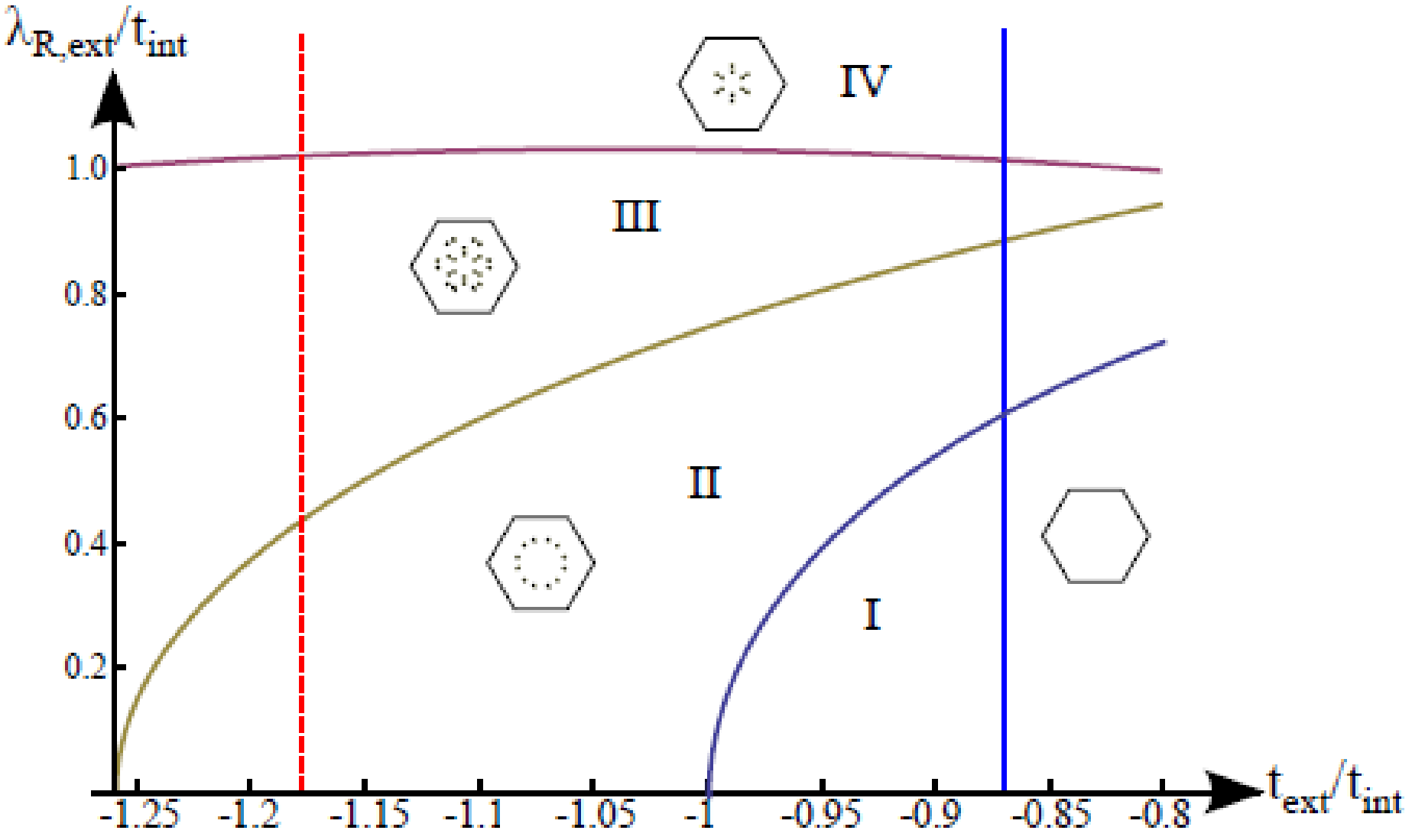
$$t_{\mathrm{ext}}/t_{\mathrm{int}} = -1.18$$



Increasing external Rashba

Rashba SOC in β/γ-graphyne

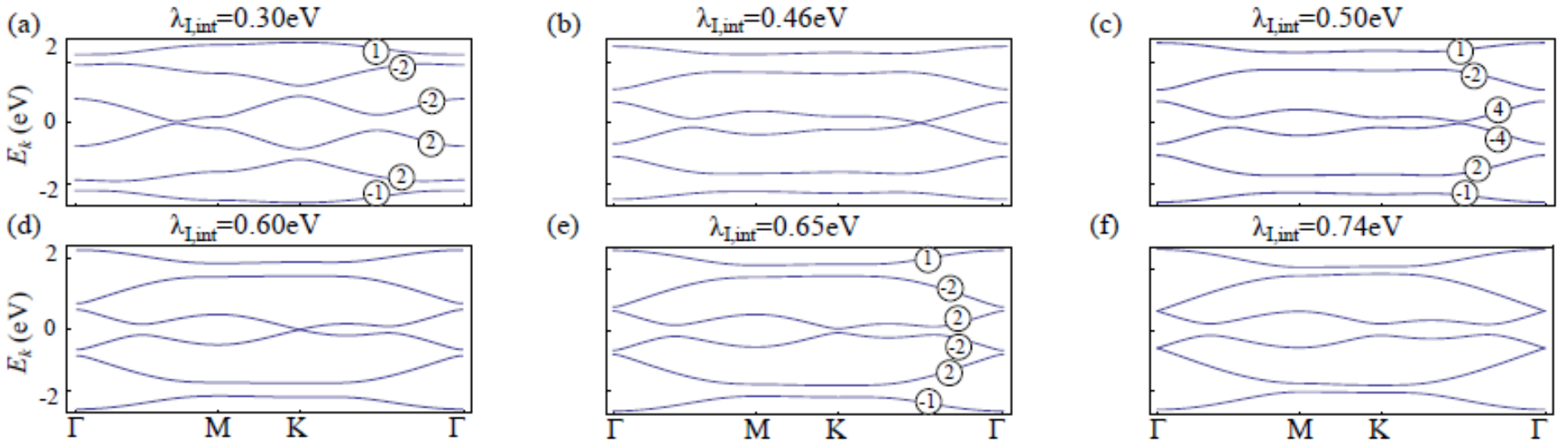
GvM, V. Juričić, and C. Morais Smith arXiv:1409.0388



Intrinsic SOC in β-graphyne

- Trivial or topological gap?

$$t_{\mathrm{ext}}/t_{\mathrm{int}} = -1.18$$



- Corresponds to QSHE

Conclusions

- Very general method to address SOC in planar carbon structures
- External and internal SOC
- In β(γ)-graphyne the internal(external) Rashba can open(close) a gap
- β-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)