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Atomic scale control and visualization of topological quantum phase transition in π -conjugated polymers driven by their length

Using topological band theory and by means of density functional theory, tight-binding and GW calculations, we can show that polymers near the topological transition point can transition from a trivial quantum phase to a non-trivial one. This transition between two insulators must proceed via closure of the electronic gap.

By employing on-surface synthesis with custom-designed precursors on a pristine Au(111) surface, we produce polymers which consist of 1D, linearly-bridged acene moieties. These polymers feature narrow bandgaps (being in the proximity of the transition point) and in-gap zero-energy edge states, when in the topologically non-trivial phase close to the topological transition point. We also reveal the important role played by a polymer's length in order to achieve an atomic scale control over the quantum phase transition between the two different topological quantum classes in one of the polymers[1-3].

References:

- [1] Sánchez-Grande, A. et al. *Angew. Chem. Int. Ed.* 58, 6559 (2019).
- [2] Cirera, B., Sánchez-Grande, A., de la Torre, B. et al. Tailoring topological order and π -conjugation to engineer quasi-metallic polymers. *Nat. Nanotechnol.* 15, 437–443 (2020).
- [3] Gonzalez Herrero, H. et al. Atomic scale control and visualization of topological quantum phase transition in π -conjugated polymers driven by their length. arXiv preprint arXiv:2105.00025 (2021)

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