Twisting between topological phases in 1D conjugated polymers

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In recent years it has become possible to tailor, with atomic precision, topologically protected states in carbon nanostructures like graphene nanoribbons[1] or 1D conjugated polymers (1DCPs).[2] Though different means have been proposed to tune trivial and non-trivial topological phases in such nanomaterials, such as hydrogenation[3] or electric fields,[4] aryl ring twist angles have not yet been considered. However, ring twisting has been shown to enable external control over electron pairing in 2D conjugated polymers via, for example, uniaxial strain.[5] Here, via accurate first principles density functional theory simulations, we demonstrate that aryl ring twist angles may indeed be used to transit from the trivial to non-trivial phases in 1DCPs made of triarylmethyl (TAM) units. Interestingly, we find that the quantum transition between the phases goes through an antiferromagnetic multiradical state displaying a finite bandgap. Thus, aside from establishing a connection between aryl ring twist angles and topology, we also demonstrate, for the first time in a carbon nanostructure, that the topological quantum phase transition may occur without bandgap closure, highlighting TAM 1DCPs as exotic topological nanomaterials.[6]

References

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Figures

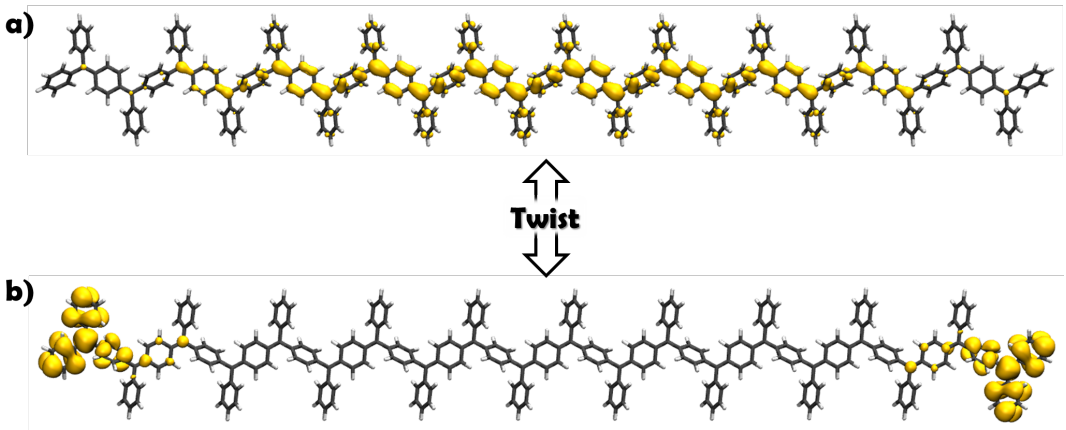

Figure 1: Spatial distribution of the highest-occupied wave-functions in TAM 1DCPs, where one may switch from **a)** the trivial phase to **b)** the non-trivial phase via aryl-ring twisting.