

## Topology-Driven Molecular Electronics Lacking $\pi$ -Conjugation

Ganna Gryn'ova<sup>a</sup> and Clemence Corminboeuf<sup>b</sup>

<sup>a</sup> Heidelberg Institute for Theoretical Studies, Germany, <sup>b</sup> École polytechnique fédérale de Lausanne, Switzerland  
ganna.grynova@h-its.org

Is  $\pi$ -conjugation necessary to achieve efficient transport in molecular electronics? In this work we use Non-Equilibrium Green's Functions technique coupled with Density Functional Theory to demonstrate how molecular topology can be used to boost the tunneling transport in single-molecule junctions featuring saturated hydrocarbon bridges.<sup>1</sup> Specifically, caged saturated hydrocarbons offering multiple  $\sigma$ -conductance channels afford transmission far beyond what could be expected based upon conventional superposition laws, particularly if these pathways are composed entirely from quaternary carbon atoms. Computed conductance of molecular bridges based on carbon nanowires, e.g., polytwistane, is not only of appreciable magnitude; it also shows a very slow decay with increasing nanogap, similarly to  $\pi$ -conjugated wires (Figure 1).

Conventional approaches to highly conductive single-molecule junctions involve  $\pi$ -conjugated systems with appropriately tuned energy levels of the frontier molecular orbitals. Our findings put forward an alternative strategy for modulating the transport in unimolecular electronics that is based on molecular topology and succeeds even in systems completely lacking  $\pi$ -conjugation, e.g., carbon nanowires, diamondoids and graphane derivatives.

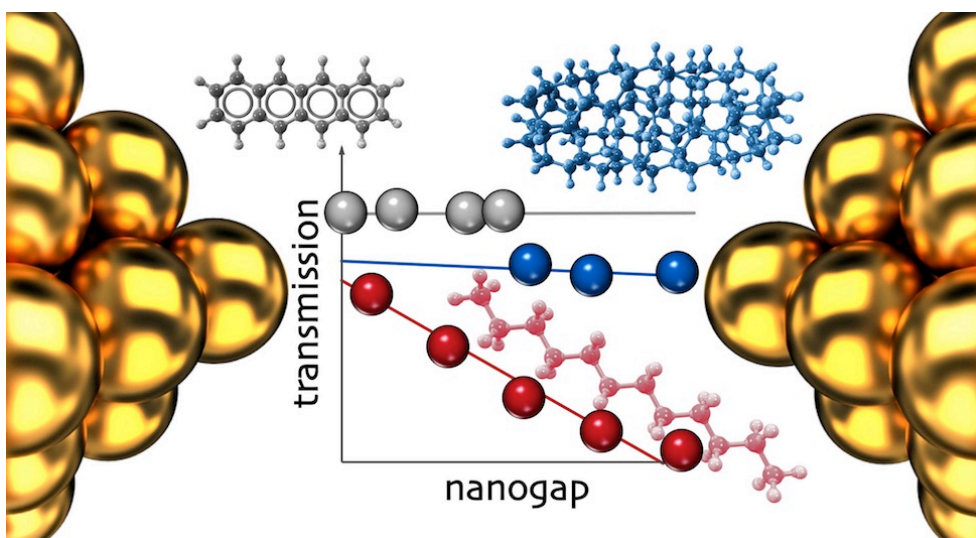


Figure 1. Computed junction transmissions vs. increasing molecular lengths.

### References

1. G. Gryn'ova and C. Corminboeuf, *J. Phys. Chem. Lett.* **10** (2019), 825.