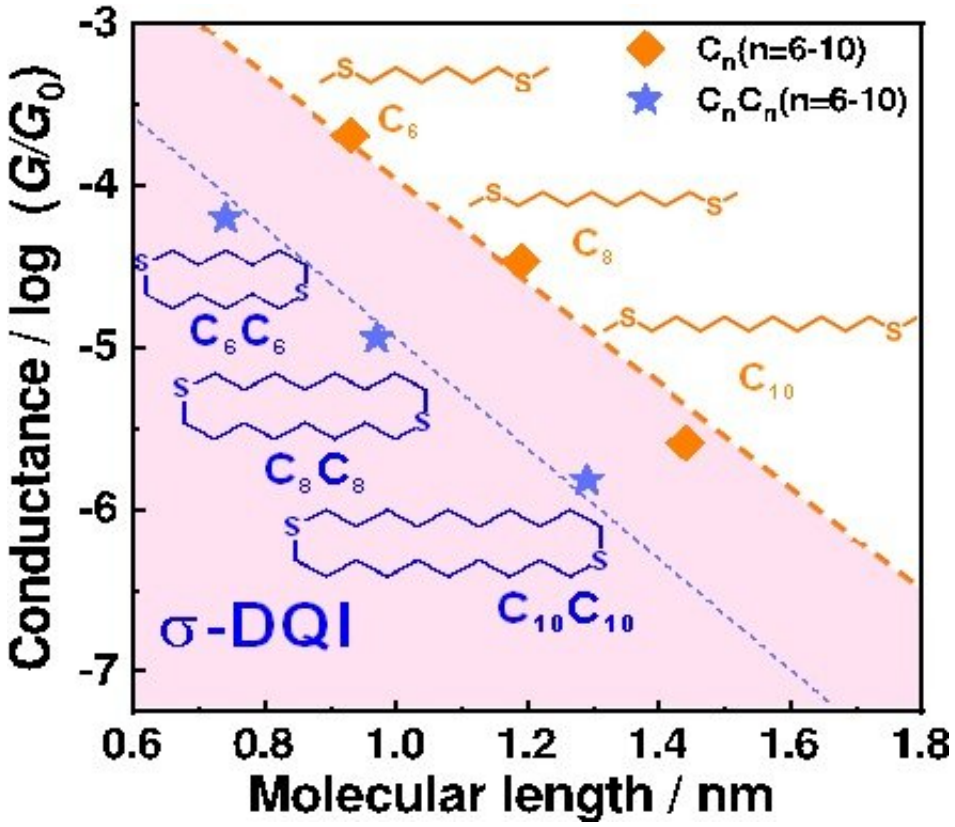
Highly insulating alkane rings with destructive σ-interference

August 16 2022



The blue star signs of saturated alkane rings show exponentially decay conductance and the decay trend is similar to saturated alkane chains, which is presented by orange squares. The alkane rings are more insulating than alkane chains when compare the identical molecular length. Credit: Science China Press

Destructive quantum interference (DQI) provides the possibility to significantly suppress the leakage current in the OFF state of molecular

devices. However, the DQI in π-conjugated molecules cannot exhibit ultralow conductance due to the existence of covalently bonded σ-transport channels.

Thus, suppressing the σ-contribution via σ-DQI is essential. In this work, researchers proposed the symmetric alkane ring C_nC_n (n = 6, 8 or 10) molecules, which were synthesized, and the corresponding electrical properties were measured.

Comparing the results with the alkane chain C_n (n = 6, 8 or 10) molecules, the alkane rings show lower conductance which contradicts the conductance superposition law in multi-channeled systems. Combined theoretical calculations reveal that the gauche conformation in a shorter chain fixed by another chain leads to decreased conductance in alkyl rings, which originates from the phase-coherent tunneling and DQI in σ-conjugated systems.

The finding suggests that through appropriate conformation locking by cyclization, the covalent alkane system can exhibit DQI, which offers strategies for future designs of molecular electronic devices and materials.

This study was led by Dr. Junyang Liu and Prof. Wenjing Hong from Xiamen University. The molecular synthesis was done by Prof. Zhong-Ning Chen (State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences) and the theoretical calculation was processed by Dr. Ali Ismael and Prof. Colin Lambert (Lancaster University).

The research was published in *Science China Chemistry*.

More information: Jingyao Ye et al, Highly insulating alkane rings with destructive σ-interference, *Science China Chemistry* (2022). DOI:

10.1007/s11426-022-1341-y