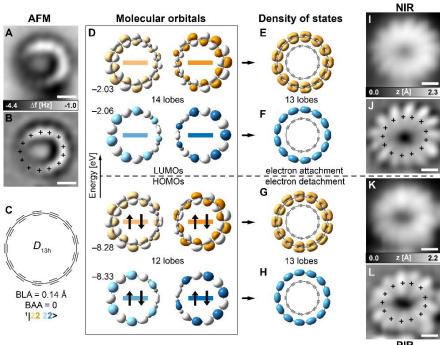
Generation and Characterization of Cyclocarbons

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The family of carbon allotropes was expanded by tip-induced synthesis and on-surface characterization of cyclo[N]carbons, C_N, molecular rings composed of N carbon atoms [1-3]. Cyclocarbons possess two orthogonal delocalized pi-systems and can undergo different Jahn-Teller distortions rendering them excellent systems for benchmarking theory [4-6]. Because they are monocyclic, they are valuable in the context of aromaticity. Even-N cyclocarbons can be doubly aromatic [1, 3] or doubly antiaromatic [2], and can exhibit polyynic [1, 2] or cumulenic [3] structures. Odd-N cyclocarbons [5], e.g., C₁₃ [7] cannot adopt a complete polyynic structure, might be open-shell systems and might feature localized carbene centres.



Cyclo[26]carbon, C₂₆, on monolayer NaCl on Au(111), generated from two C₁₃ precursors. (A) AFM and (B) Laplace-filtered AFM data, with the positions of short bonds marked. (C-H) gas-phase DFT calculations. (I, J) STM at V = 2.0 V, (K, L) STM at V = -2.75 V. (J, L) Laplacefiltered images of (I, K) with the positions of the short bonds (from B) marked. Experiments with CO-tip functionalization. Scale bars 5 Å. [7]

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References

- [1] K. Kaiser et al. Science 365, 1299-1301 (2019)
- [2] Y. Gao et al. Nature 623, 977–981 (2023)
- [3] L. Sun et al. Nature 623, 972–976 (2023)
- G. V. Baryshnikov et al. J. Phys. Chem. A 124, 10849–10855 (2020) [4]
- [5] G. V. Baryshnikov et al. J. Phys. Chem. A 126, 2445-2452 (2022)
- I. Rončević et al. J. Am. Chem. Soc. 145, 26962–26972 (2023) [6]
- F. Albrecht et al. preprint: 10.26434/chemrxiv-2023-ddrh7-v2 (2024) [7]