Superhydrogenation of pentacene: the role of zigzag-edges in H_2 formation

D. Campisi[1], F. D. Skødt Simonsen[2], A. Candian[1], R. Martinazzo[3], L. Hornekær[2], A. G. G. M. Tielens[1]

[1]Leiden Observatory, *Leiden University, Leiden, The Netherlands*
[2]*Department of Physics and Astronomy, Aarhus University, Aarhus, Denmark*
[3]*Department of Chemistry, Milan University, Milan, Italy*
campisi@strw.leidenuniv.nl

Investigating the hydrogenation of carbonaceous materials is of interest in a wide range of studies, including electronic device development, hydrogen storage optimization, and in particular astrocatalityc formation of molecular hydrogen in the universe. Polycyclic Aromatic Hydrocarbons (PAHs) are ubiquitous in space, locking up close to 15% of the elementary carbon. They contribute to the ionization balance and heating of interstellar gases, as well as the formation of complex molecular species [1]. Experiments and theory have also shown that PAHs are an important player in the formation of cosmic molecular hydrogen (H_2) [4, 5].

Studies making use of density functional theory (DFT) have shown there to be a preference for particular carbon sites when an atomic hydrogen is attached to pentacene [2], further the hydrogenation requires a change to the aromatic structure of these organic compounds and is therefore associated with high energy barriers. Understanding the chemical dynamics of super-hydrogenated pentacene, and in particular the hydrogenation sequences which leads to the so-called “magic number” sequence detected in mass spectra, is indispensable for shedding light on the existence of borderline aromatic-aliphatic behaviour of PAHs, as well as for the observation of potential magic numbers in the interstellar population of super-hydrogenated PAHs.

In this work we use DFT [6] to estimate the binding energies and sticking barriers, and in this way we can determine the number of additional hydrogen atoms that would readily attach to pentacene. Results are rationalised with simple concepts that apply equally well to different PAHs, and provide the hydrogenation sequence most likely followed by the molecule in a hydrogen rich atmosphere.

References:
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