

Synthesis, Nanostructural and Electronic Characterization of Anthracenedicarboximide Derivatives.

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Since the discovery of the first semiconducting organic molecules, great interest has been paid to the field of organic semiconductors. Intended to complement, rather than to replace their inorganic counterparts, organic molecules have several important advantages, not least of which is their tunability. Indeed: colour, morphology, solid-state packing as well as many other properties can be finely modulated in target molecules by slightly varying their structure. What is more, it is usually possible to cheaply process these materials at low temperature (typically below 250°C), allowing for a wide range of potential applications and avoiding the costly microfabrication rooms now eponymous with the semiconductor industry.

Despite a host of suitable p-channel candidates (which conduct charge via holes), organic n-channel materials (where charge carriers are electrons) are rare and usually suffer from electron-trapping defects, particularly when exposed to air. One strategy to circumvent this trapping has been the incorporation of strongly electron-withdrawing groups along a semiconductor's π -conjugated core, in order to stabilize electrons as they traverse the material. Anthracenedicarboximides (ADCIs) are one such n-type semiconducting material, in which carboximide groups at either end provide the electron-withdrawing effect necessary for a low LUMO. ADCIs are an ideal candidate for an organic semiconductor, thanks to their flat core (allowing efficient packing in space) and their symmetry (allowing for easy functionalization) [1].

We have thus completed a Density Functional Theory computational study of the ADCI class of molecules, in order to calculate electronic levels and reorganization energies of several compounds. As a result, we have identified and synthesized a considerable number of ADCI derivatives.

We will present synthesis, TFT performance and self-assembly properties of the parent (unsubstituted) ADCI **1** (cf. figures 2 and 3) in addition to that of several novel derivatives, complemented by DFT calculations of the electronic levels and reorganization energies. The specific goal of the study is to probe the effects of ADCI side groups on surface nanostructure and, therefore, on molecular packing and charge mobility. We will also investigate whether alkyl chain length parity plays a role in this system.

Significantly, the results of this study will develop a new type of n-type semiconductor. Additionally, we will advance the current understanding of the relationship between molecular structure/crystal packing and device performance in n-channel materials, allowing for more rational design.

References

[1] Wang, Z.; Kim, C.; Facchetti, A.; Marks, T. J. *J. Am. Chem. Soc.* **44** (2007), 13.

Figures

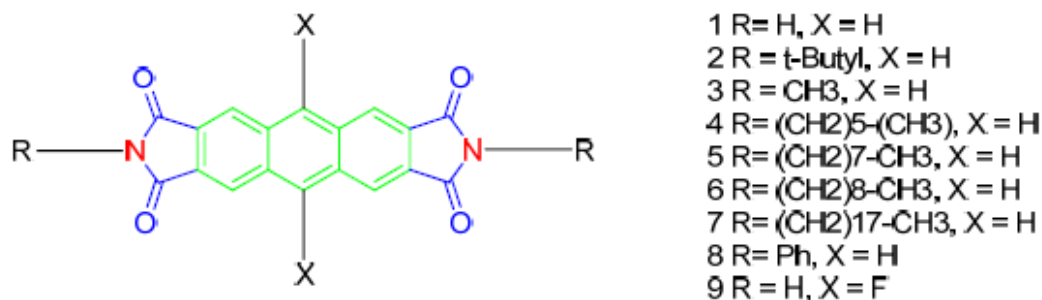


Figure 1 - Summary of compounds synthesized and studied

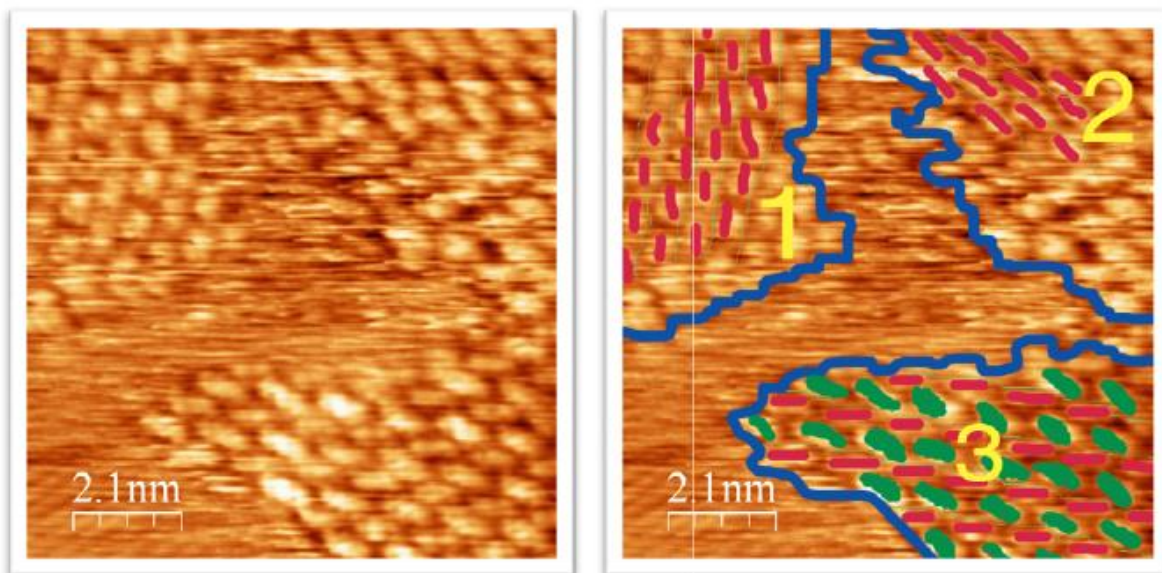


Figure 2 - STM image of 2-D SAMN formed from compound 1 at the heptanoic acid/HOPG surface. The processed image at right was marked up to show distinct domains.

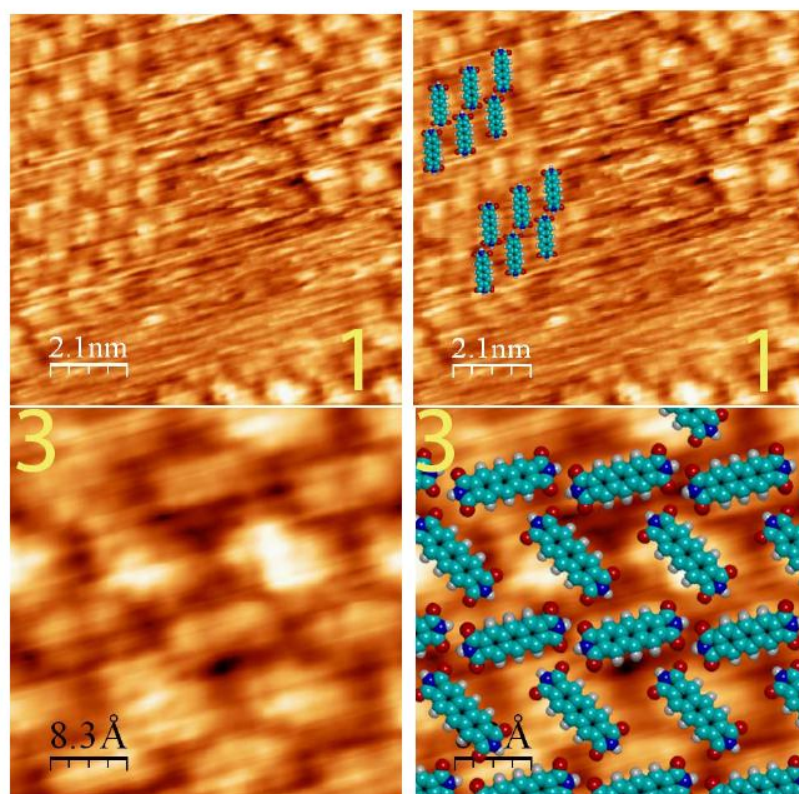


Figure 3 – Enlargements of domains 1 and 3 of the STM images from Figure 2, with DFT-optimized molecular models of the molecules superimposed on the image.