Self-organized, linear hydrocarbons as a major source of surface contamination on van der Waals materials

András Pálinkás¹

György Kálvin¹, Konrád Kandrai¹, Gergely Németh², Miklós Németh³, Áron Pekker², József S. Pap³, Péter Petrik¹, Katalin Kamarás², Levente Tapasztó¹ and Péter Nemes-Incze¹

¹Centre for Energy Research, Institute of Technical Physics and Materials Science, 1121 Budapest, Hungary

²Wigner Research Centre for Physics, 1121 Budapest, Hungary

³Centre for Energy Research, Institute for Energy Security and Environmental Safety, 1121 Budapest, Hungary

andras.palinkas@ek-cer.hu

There is a rule of thumb in surface science which says: 'Once a freshly prepared, clean surface is brought out from UHV to open lab air, it becomes contaminated with water, hydrocarbons, other vapors, etc.' Here we show by complementary, high-resolution atomic force (PeakForce QNM and LFM) and scanning tunneling microscopy (STM) that after a few days of exposure to ambient air, a self-organized, crystalline lattice of molecules is formed on the surface of van der Waals (vdW) materials. The molecules self-organize into parallel stripes with 4 ± 1 nm periodicity on several, distinct surfaces: graphene, graphite, hBN, MoS₂. By low-temperature STM measurements, we have resolved the atomic structure of the molecules on graphite (see Fig1c) and in combination with infrared spectroscopy, we reveal that the molecules are linear, saturated hydrocarbons with a length of 20-24 atoms (see Fig2), most likely normal alkanes. We show a direct causal link between the selforganized stripe structure of the molecule layer and the well-known [1], but yet unexplained friction anisotropy domains measured on vdW materials (see Fig1a-b). Additionally, we found that the local orientation of the molecular layer can be switched on purpose between the three distinct zigzag crystal directions. Repeated scans along the desired direction by contact mode AFM enables the redrawing or "nano-patterning" [2] of the friction domains on vdW-materials. Beyond the manipulation of the molecular lattice, we show details of the growth dynamics and the controlled desorption through annealing. Our work is a major step towards understanding the origin of the ubiquitous hydrocarbon contamination on vdW crystals and its effects on their measured properties.

References

- [1] Gallagher, P. et al. Nat. Commun. 7 (2016) 10745
- [2] Verstraete, L. & De Feyter, S., Chem. Soc. Rev. 50 (2021) 5884–5897

Figure 1: a) Parallel stripes of 4 nm periodicity on the surface of a graphene/hBN heterostructure (PeakForce AFM Topography). **b)** Friction force signal of the same region as in a). **c)** Low temperature STM image of the airborne monolayer on graphite.