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Tuning the electrode work function by deposition of chemically functionalized MXenes-an SPM study

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Graphene has triggered a great interest in the promising world of two-dimensional (2D) materials: thanks to their chemical and physical properties, this new class of compounds is expected to be employed in several applications in future and emerging technologies addressing numerous societal needs, such as faster and better performing electronics, as well as energy storage and conversion. Following the success of graphene, MXene, a new family of 2D transition metal carbides/nitrides/carbonitrides, has recently attracted considerable attention due to its combination of excellent metallic conductivity and rich surface chemistry features. Independent from its high conductivity, the variable surface chemistry make MXene unique for photo-/electronic applications [1].

In this study, MXenes, in their pristine form as well as chemically-functionalized with different organic molecules, are studied with atomic force microscopy to understand their morphology and with Kelvin probe force microscopy (KPFM) [2] to monitor the changes in the work function of different substrates after their deposition on them (Fig. 1 and 2). The possibility to tune the work function of MXenes and/or of different surfaces by chemical functionalization is expected to be of key importance for many applications, including energy harvesting and conversion [3]. Combining KPFM with macroscopic Kelvin Probe we are able to understand the origin of these changes.

References

[1] Yury Gogotsi and Babak Anasori, The Rise of MXenes, *ACS Nano* **2019** *13* (8), 8491-8494
[2] V. Palermo, M. Palma, and P. Samorì, *Electronic Characterization of Organic Thin Films by Kelvin Probe Force Microscopy* (2006), In Scanning Probe Microscopies Beyond Imaging, P. Samorì (Ed.).
[3] Agresti, A., Pazniak, A., Pescetelli, S. *et al.*, Titanium-carbide MXenes for work function and interface engineering in perovskite solar cells., *Nat. Mater.* **18**, 1228-1234 (2019)

Figures

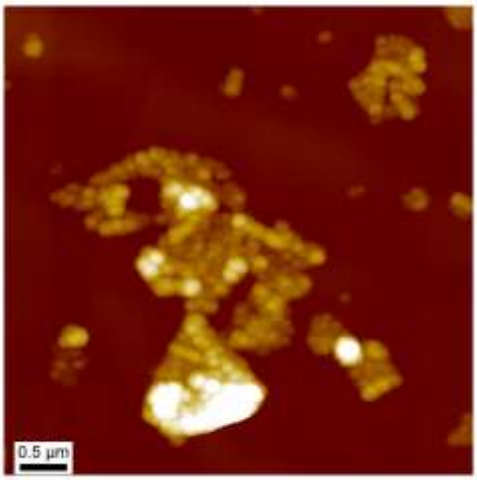

Figure 1: Topography of functionalized MXenes on HOPG substrate.

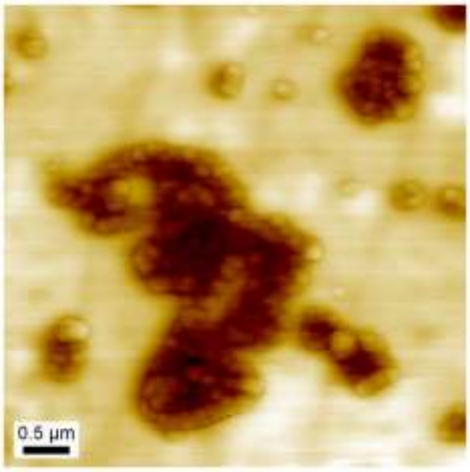

Figure 2: Corresponding surface potential difference of functionalized MXenes on HOPG substrate.