Fundamental processes at 2D materials: From in-situ growth studies to a single-molecular perspective of water dynamics.

P. Maier[1], N. J. Hourigan[1], A. Ruckhofer[1], M. Sacci[2], A. Pyane[2], A. Tamtögl[1]

[1] *Institute of Experimental Physics, Graz University of Technology, Graz, Austria*
[2] *Department of Chemistry, University of Surrey, Guildford, United Kingdom*

tamtoegl@tugraz.at

Starting from recent findings about the growth of two-dimensional (2D) materials such as hexagonal boron nitride (h-BN) via chemical vapour deposition (CVD) I will discuss how helium atom scattering (HAS) can be used to determine surface properties of 2D materials. E.g., in the case of h-BN I will illustrate how intermediate structures during the growth of h-BN from borazine molecules can be observed [1]. As illustrated in the Figure, a gas-phase precursor is deposited on a solid substrate, diffuses, dehydrogenates and eventually attaches to a growing 2D cluster. The complex process involves several steps but has so far only briefly been discussed in the context of graphene formation.
Furthermore, the lineshape broadening upon inelastic scattering from surfaces can be used to determine the characteristics of molecular diffusion. Using this technique, we have studied the diffusion of water on the surfaces of Dirac materials (graphene and the topological insulator Bi_2Te_3)[2-4]. Thus, we can specify the mechanisms underlying the motion of water and, by comparison with first-principle calculations, we identify aspects of its adsorption geometry, as well as the energy landscape for the motion. Together with *ab-initio* calculations we illustrate that despite a similar lattice structure of h-BN compared to graphene, the motion of water on h-BN exhibits a completely different behaviour [2]. In contrast to a high adsorption energy, an extremely low diffusion barrier is present, giving rise to motion with a strong normal component / “easy” change of the molecular H_2O orientation with respect to the surface. The dynamics thus involve a rearrangement of the water molecules with a large z-dependence of the hydrogen atoms in addition to the lateral motion. Moreover, unlike graphene, h-BN is an electrical insulator, and we will further discuss these findings in light of previous reports about quantum friction.

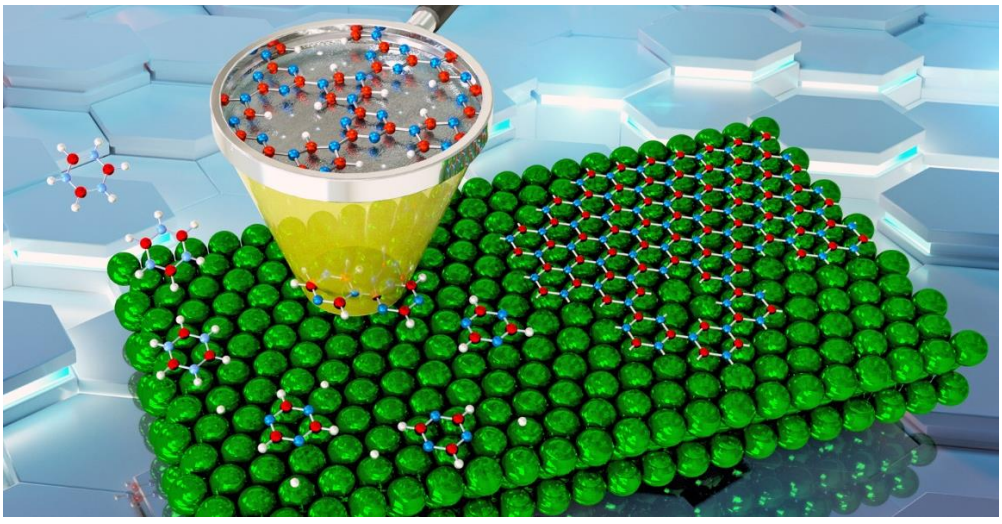

Fig. 1. How to make 2D materials with tailored holes: New open network structures have been discovered in a combined helium scattering and DFT study, during on-surface synthesis of hexagonal boron nitride.

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[4] A. Tamtögl *et al.*, Nat. commun., **11**, 278 (2020).