ADVANCED MATERIALS SCIENCE

Fields of Expertise TU Graz

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Source: Lunghammer – TU Graz

The FoE Advanced Material Science is happy to share several good pieces of news regarding some of its members. A new EIC (European Innovation Council) Pathfinder project coordinated by Stefan Spirkhas been approved. It will deal with the development of vanillin-based redox cells. In addition, a new paper from the experimental physics team led by Martin Schultze and Markus Ossiander was published in the journal "Science". The paper is entitled "Extreme ultraviolet metalens by vacuum guiding".

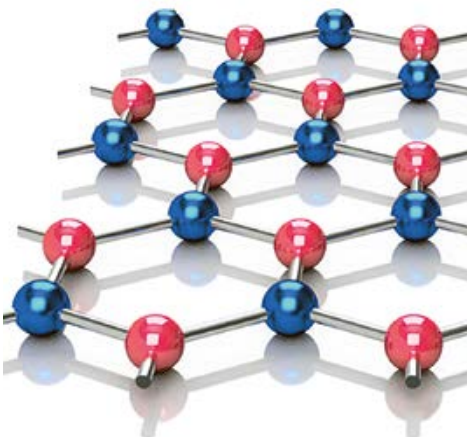
The 19th call of the initial seed funding of TU Graz was very successful for the FoE Advanced Material Science since all the submitted projects were able to be funded! The awardees were:

- Rudolf Vallant with a proposal on "Embrittlement – efficient and reliable testing of steels"
- Markus Koch with the proposal "Real-time observation of charge and energy flow in nanomaterials"
- Markus Ossiander who proposed "Extreme ultraviolet light in opaque media"
- Simon Hollweger with the proposal "Quantum corral surface state design"
- Ulrich Hirn with a proposal called "Infinite paper" in collaboration with TU Darmstadt

We wish them good luck in their proposal submissions, and we look forward to more submissions at the next call.

Anton Tamtögl

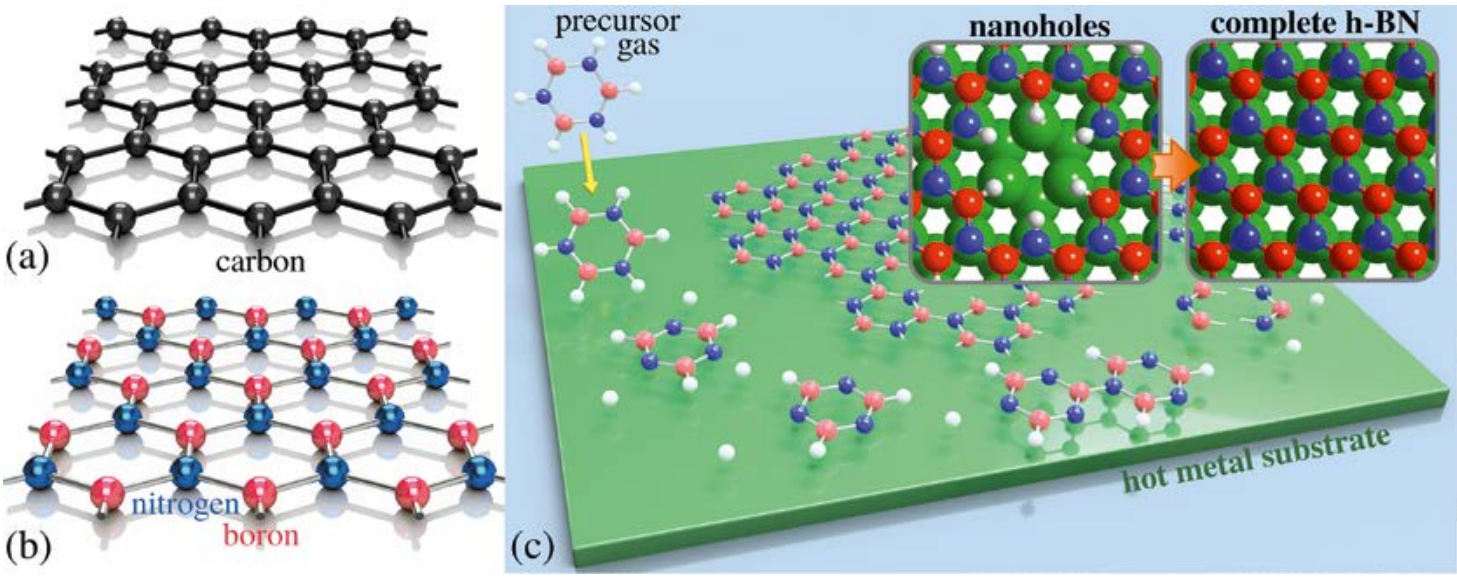
Probing the Formation of Nanomaterials and the Motion of Single Water Molecules



The growth of nanostructures and two-dimensional materials requires understanding and control of each step to tailor their properties for specific applications. Similarly, the interaction of novel materials with water holds implications, from technological applications to fundamental physics and chemistry on Earth as well as in space. Due to challenging experiments, these details are just starting to unfold.

In materials science, two-dimensional (2D) materials with only a single-atom thickness, are an emerging class of systems with exotic properties and a wide range of emergent applications. Graphene is the most famous 2D material, where carbon atoms form a 2D honeycomb crystal structure (Figure 1(a)). Similar to graphene, hexagonal boron nitride (h-BN) also exhibits a honeycomb structure, as shown in Figure 1(b), but with alternating boron and nitrogen atoms replacing the carbon atoms of the hexagon. For this reason it is sometimes also called white graphene. h-BN finds applications in several microelectronic and nanotechnology applications, including photonic and power devices, fuel cells and as dielectrics for field-effect transistors.

Atomically thin 2D materials are grown by breaking down gas on a hot metal surface, but while the evolution of these 2D materials via on-surface synthesis requires understanding and control of each step during the growth process, due to the high temperatures and fast conversion it is extremely difficult to observe the process. As illustrated in Figure 1(c), h-BN is grown by exposing a metal surface to a >



specific gas (borazine). Like structures formed of individual Lego bricks, the gas consequently decomposes on the hot metal substrate and forms the desired 2D material. Naturally, there are several intermediate steps involved before the 2D material is completed but these have gone unnoticed up to now due to the mentioned experimental difficulties.

In a study published in Nanoscale Horizons [1], the surfaces group at the Institute of Experimental Physics at TU Graz has recently been able to monitor the growth of h-BN. As illustrated in the inset of Figure 1(c), the hexagonal precursor gas first gets rid of the hydrogen atoms attached to nitrogen and the individual hexagonal rings join each other at these positions, leaving a network of nanoholes behind. Only by placing an increasing number of gas molecules at sufficiently high temperature at the surface do these holes finally get filled up, by which time the entire 2D material is completed.

The main impact of our study is that it addresses the route from the gas-phase precursor to the complete 2D material rather than just focusing on the end-product; this holds broader implications for other 2D materials and the field of nanostructures which may be employed for novel advanced materials. Consequently, our study appeared on the journal cover – see Figure 1(d) and was among the most read articles of 2022.

As a second line of research, our group is not only interested in the formation of 2D materials and nanostructures but also in the mobility and motion of individual atoms and molecules on these surfaces. The study of these surface dynamical processes is a unique and challenging problem for experiments, as it requires both sub-nanometre spatial resolution (Figure 2) and fast (picosecond) temporal resolution (Figure 3(b)).

Despite the microscopic motion of water being a central question in catalysis, biophysics, etc. or in technological applications such as tailored surface coatings, experiments are particularly rare due to the mentioned challenges. In that context we have recently published a review article which covers recent progress regarding the atomic-scale details of water, specifically on 2D materials [2]. The slow and difficult progress in determining the properties of water molecules on surfaces is due to two main factors: I) Strong hydrogen bonding between water molecules as shown in Figure 3(b) causes the rapid formation of water clusters and islands almost immediately upon water exposure onto solid surfaces and microscopic techniques are not suitable to investigate surface dynamics operating in the picosecond timescale (Figure 2(b)). II) Water on surfaces forms a wide variety of conformations which easily interchange from one to another upon motion and the formation of these hydrogen bonds. In addition to the experimental challenges, these structures have only recently been accessible by theoretical i.e. computational methods.