Advanced Lab / Master Thesis

Prof J. P. Rabe, Prof N. Koch, Prof C.-A. Palma

Hydrogenating nanographenes *en route* to atomically-precise nanodiamond

Keywords: UHV, AFM, STM, XPS, **DFTB**, Raman, Plasma

Update: Online Advanced Lab & remote supervision option available

Fully hydrogenated graphene (*Science*, 323 (5914), 610-613, **2009**), is expected to possess hole-doped superconducting critical temperature (T_c) one order of magnitude higher than diamond, above 90 K (*Phys. Rev. Lett.*, 105, 037002, **2010**). However, its challenging fabrication makes alternative nanomaterials such as nanographanes attractive for real-world applications. Here, you will help in the discovery of nanographane (**Figure 1**) and continue with the first steps towards nanodiamond fabrication from nanographane, a material of potential relevance in quantum computing. In collaboration with Prof Müllen (**Mainz**).

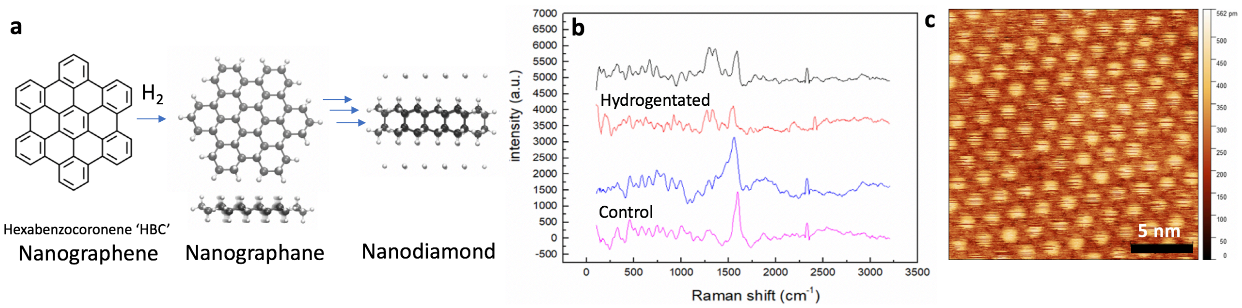

Figure 1. a Hydrogenation of HBC for nanographane and possibly nanodiamond formation. **b** Raman and **c** STM of hydrogenated HBC

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Stacking of molecular heterostructure photoresists toward atomically precise 3D printing of nanomembranes

Keywords: UHV, AFM, STM, XPS, **MD**, Raman, Photophysics

Update: Online Advanced Lab & remote supervision option available

Stacking 2D-material heterostructures is a promising method for composing the next generation of advanced materials (*Nature*, 499, 419–425, **2013**). Their supramolecular heterostructure counterparts are largely unexplored materials capable of bearing photopatternable units (*J. Am. Chem. Soc.*, 136, 12, 4651-4658, **2014**) for 3D printing down to the molecular scale. We have demonstrated 2-, 3-layer porphyrin stacks (**Figure 1**) and your project will deal with the further study a photoactive layer via physical vapor deposition under ultra-high vacuum and AFM characterization.

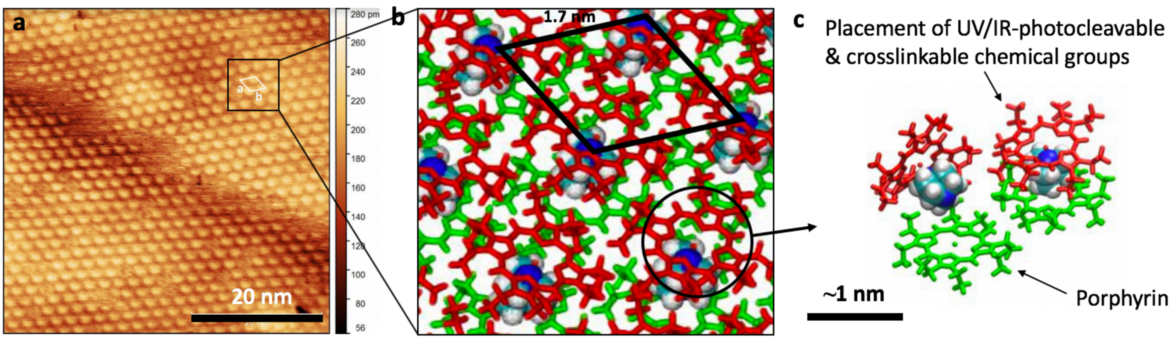

Figure 1. a AFM of crystalline porphyrin architecture on Au(111) and **b, c** Target third layer, potentially photoactive porphyrin

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Photodoping of graphene and diamond C(100) by graphene nanoribbons

Keywords: AFM, STM, **TD-DFTB**, Raman, Device, Photophysics

Update: Online Advanced Lab & remote supervision option available

Doping graphene results in a dramatic change of its photophysical properties for advanced photomodulators, photovoltaics and transistor logic (*Science* 320 206-9, **2009**). We have shown how graphene nanoribbons can be studied on diamond C(100) substrates (*J. Am. Chem. Soc.*, 140, 25, 7803-7809, **2018**) collaborating with Prof Sanchez and Prof Frauenheim (**Bremen**) to demonstrate how "cove" graphene nanoribbons (CGNRs) tune the IR-UV-Vis optical spectrum of graphene and diamond (**Figure 1**). Here, your will study the effect of chemical doping on graphene via Raman and IR-UV-Vis spectroscopy in collaboration with Prof Narita and Prof Müllen (**Mainz**).

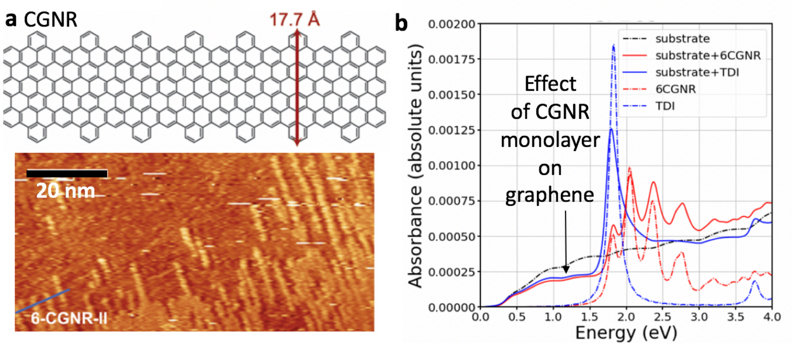

Figure 1. a STM data of "cove" graphene nanoribbon (CGNR) on diamond H-C(100) and **b** Simulated absorbance spectrum of CGNR on graphene

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Phonon topology in molecular architectures

Keywords: AFM, STM, Raman, MD, **DFTB**, **Phonotopy**

Update: Online Advanced Lab & remote supervision option available

The Nobel Prize in Physics was awarded in 2016 for the *discovery of topological phases of matter*. We recently showed, employing classical atomistic calculations, that the edges of a chiral supramolecular nanoribbon can host topological edge phonon states (**Figure 1** and *J. Phys. Chem. Lett.*, 10, 19, 5830-5835, **2019**). In this project, you will establish your online database, employ molecular dynamics (MD) and STM at the solid-liquid interface, to study various molecular architecture patterns which can host topological phonon bands, toward supramolecular thermal waveguides, thermal diodes, and thermal logics.

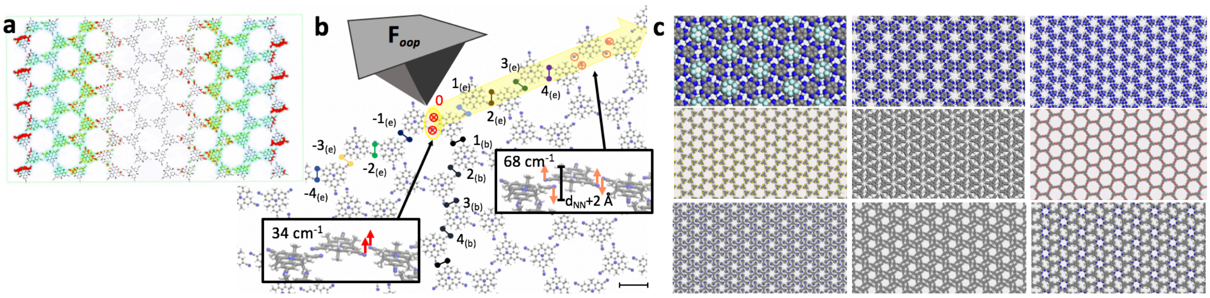

Figure 1. a Chiral phonon map in a supramolecular ribbon **b** Simulated excitation of a chiral phonon **c** Available experimental systems

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