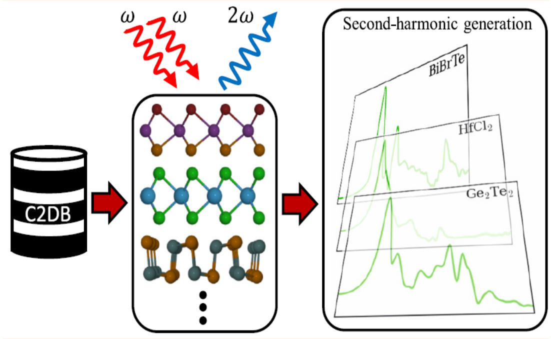
Center for Nanostructured Graphene - Highlights in 2021

A Library of 2D materials for Nonlinear Optics



If a light source is sufficiently intense, the optical response of materials under illumination is nonlinear. This leads to host of interesting henomena. In Phenomena. In particular, the color of the transmitted light may be different from different from the incident beam. An example of this is second harmonic generation, in which the optical frequency is doubled. In addition, an oscillating light beam can induce a DC current via nonlinear interactions. Apart from the exciting fundamental physics revealed by these processes, several applications in optical communication and signal processing rely on nonlinear optics. In a recent paper, members of CNG have examined 375 2D materials in order to identify promising candidates having large nonlinear response. We have used state-of-the-art theoretical tools to predict the nonlinearity of materials selected from the C2DB database. In this manner, several highly promising structures have been suggested. Moreover, some interesting general trends have been identified. First, we find that the band gap of the material is a crucial indicator for the response. Secondly, certain atomic constituents such as chromium seem to boost the nonlinearity. Finally, we have shown that our most promising candidates are close the theoretical upper limit implied by fundamental quantum mechanical rules. If verified experimentally, these findings could pave the way for significant advances in nonlinear optical devices based on 2D materials.

A. Taghizadeh, K. S. Thygesen and T. G. Pedersen, "Two-dimensional materials with giant optical nonlinearities near the theoretical upper limit", ACS Nano 15, 7155 (2021).

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2D materials cut closer than ever by anisotropic etching

Precise nanopatterning of 2D materials is one of the key routes to functionalize 2D materials for new types of electronics and nanophotonics. This is also a key focus of CNG. To fully exploit quantum properties, such as the spin and valley degrees of freedom for new electronic components, we need to be able to pattern 2D materials with a resolution below 10 nm, approaching the atomic scale.
At CNG, we have worked intensely miniaturizing nanostructures in 2D layers based on electron beam lithography and reactive ion etching. We have demonstrated that anisotropic reactive ion etching can be used realize sub-10 nm features in 2D crystals. We used sulfur hexfluoride (SF_6) plasma to etch multi-layer hexagonal boron nitride (hBN) and four different multi-layer transition dichalcogenides (TMDs). The TMDs exhibited varying degrees of anisotropic etching, where circular holes were etched into hexagons with sharp corners and low edge roughness. Transmission electron microscopy revealed that the etch rate is largest at armchair terminated edges and smallest at zigzag edges, leading to zigzag-terminated holes and armchair terminated protrusions.
SF6 etching in hBN resulted in constant etch angles, independent of crystal lattice orientation.This can be used to downsize and sharpen patterns defined by electron beam lithography, by placing hBN on top of another 2D crystal and using hBN as an extra etch mask. In this configuration, a lithographically defined triangular hole with rounded corners at the top of the hBN crystal will be smaller and have self-sharpened corners at the base of the hBN crystal. This makes it possible to create lithography-based nanostructures in 2D crystals with unprec-edented precision.

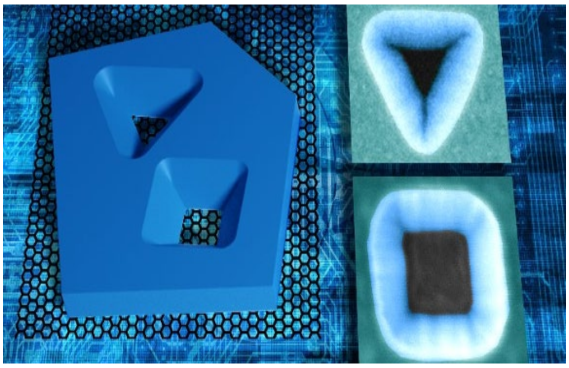

Figure 1. Left, illustration of downsizing self-sharpening effects that can be achieved by using hBN as an extra etch mask. Right, scanning electron microscopy images of holes in hBN made by electron beam lithography and sulfur hexafluoride etching.

M. Fischer, Dorte R. Danielsen, Anton Lyksborg-Andersen, Kirstine E. S. Nielsen, Bjarke S. Jessen, Timothy J. Booth, Manh-ha Doan, Yingqiu Zhou, Peter Bøggild: "Super-resolution Nanolithography of Two-Dimensional Materials by Anisotropic Etching", ACS Appl. Mater. Interfaces, 13, pp. 41886-41894 (2021).