Growth of Graphene Nanoflakes/h-BN Heterostructures

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1. Introduction

2D materials such as graphene, hexagonal boron nitride (h-BN), or transition metal dichalcogenides, and their heterostructures are gaining increasing interest because of their extraordinary properties, which can range from superconductivity to large charge carrier mobilities. In this paper, the electronic and structural modifications of h-BN on Rh(111) are investigated by the intercalation of carbon forming graphene nanoflakes between the h-BN and the Rh(111) surface. The carbon atoms—natural impurities in Rh bulk crystals—diffuse to the surface during the h-BN growth and segregate there during cooling. The graphene nanoflakes are present at particular sites under the wires of the h-BN nanomesh leading to an altered appearance of the Moiré pattern and modified electronic and chemical properties. Thus, a novel fabrication route of graphene nanoflakes located in a heterostructure on Rh(111) and h-BN is shown by steering the segregation of carbon impurities at the rhodium surface.

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h-BN-G heterostacks often utilizing high gas pressures of the precursors or gaseous catalysts.[9,11,22] Another very appealing approach is the co-segregation growth.[21,24] For example, a sandwiched substrate consisting of a film containing boron and nitrogen atoms covered with a carbon-rich Ni-film has been used.[23] It was shown that this method is wafer scalable and as such a possible route to grow h-BN-G heterostacks for industrial applications.[23]

In this article, we used a similar approach to modify the electronic properties of h-BN on Rh(111). Depending on the amount of carbon dissolved in the near-surface region of the Rh(111) either pure h-BN (low carbon amount) or a modified h-BN structure with intercalated graphene nanoflakes (here called nG-h-BN) can be grown. Our scanning tunneling microscopy (STM) and spectroscopy (STS) investigations of this phase together with density functional theory (DFT) calculations show that it exhibits significantly different electronic and chemical properties compared to the pure h-BN layer.

2. Results and Discussion

Depending on the concentration of subsurface carbon[25]—intrinsic impurities in the Rh single crystal—two different surface structures were observed when the Rh(111) single crystal was exposed to borazine. For an impurity-free subsurface depletion layer prior to borazine exposure, a pure h-BN layer was observed as reported in the literature (c.f. Figure 1a).[3] For higher carbon concentrations present close to the crystal surface (e.g., a thinner depletion layer), we observed large continuous domains of a different phase with an altered appearance when imaged with STM (Figure 1b,c). This phase will be referred to as “graphene nanoflakes/h-BN” (nG-h-BN).

The nG-h-BN phase consists of a highly ordered arrangement of star-shaped structures as visible in the large area STM image shown in Figure 1b. Investigations of nG-h-BN by high-resolution STM imaging give insight into the periodicity and the structure of the Moiré pattern (see Figure 1c). The continuous layer of nG-h-BN consists of a long-range ordered, highly symmetric Moiré structure, which has the same periodicity as the h-BN superstructure (3.14 ± 0.1 nm, see Figure S2, Supporting Information). This can also be seen by the Fast-Fourier-Transformation (FFT) patterns of the STM images, displayed in the insets in Figure 1a,b, which show a similar hexagonal pattern.

The nG-h-BN Moiré consists of areas of low apparent height with hexagonal shape (“hexagon”) and triangular shape (“dark triangle”) as well as elevated triangular regions (“bright triangles”), indicated in Figure 1c. Each hexagon is surrounded by one threefold symmetric set of dark triangles and one set of bright triangles, respectively. The high-resolution STM image shows that the dark triangles are surrounded by structures with low apparent height, which are denominated as “ribs”. Performing scans in point-contact mode[26] leads to STM images where the atomic bonds of the nG-h-BN are visible (inset in Figure 1c). These images show that the surface consists of one continuous atomic layer and does not contain structural defects such as riffs or broken bonds. This suggests that the modification of the h-BN Moiré takes place by modifying the space, that is, the interface, between the h-BN and the Rh(111) substrate. It has been already shown that hydrogen and argon can be intercalated between the metal surface and the h-BN layer.[27] A similar effect can be expected for carbon atoms diffusing from subsurface layers to the surface during the annealing and segregating between the h-BN layer and the Rh surface during the cooling that follows h-BN growth. We assume that the corrugation of the h-BN is lifted at high temperatures in accord with a recent molecular dynamics study.[28] The formation of the carbon rings underneath the rims of the h-BN takes place during the cooling process similar to the segregation-induced

![Increasing amount of subsurface carbon](image)

**Figure 1.** Different phases of h-BN on Rh(111). a) h-BN obtained on an impurity-free subsurface depletion layer on Rh(111) (U = 1.0 V, I = 100 pA); b) Overview of the nG-h-BN phase obtained with a thinner carbon surface depletion layer (U = −1.0 V, I = 50 pA); c) High-resolution image of the nG-h-BN Moiré pattern where the different structural motifs are denominated (U = 5 mV, I = 5 pA); inset: STM image acquired in point contact mode (U = 10 mV, I = 90 nA). The insets in (a) and (b) are the Fast-Fourier Transformations of STM images of h-BN and nG-h-BN, respectively.
graphene growth on Rh(111).[29] Since the observed Moiré pattern does not depend on the coverage of nG-h-BN but is the same even if the surface is almost fully covered with this structure, we assume that the growth of carbon rings underneath the h-BN is self-limiting and that the amount of carbon rings in the graphene nanoflakes underneath the bright triangles is always the same. Although the focus of this work is not on the preparation of samples containing a certain amount of nG-h-BN phase, rather it is on the structural and electronic differences between this phase and pure h-BN, we were able to grow samples with at least 90% coverage, as judged by our STM measurements.

Details of the transition from h-BN to nG-h-BN are revealed at low carbon impurity concentrations. In this situation, the emergence of isolated triangularly arranged point defects located at every other wire site of the h-BN Moiré pattern can be observed as shown in Figure 2a. STM images of areas in which pure h-BN and nG-h-BN phases are present (Figure 2b,c) indicate that there is no interruption of the h-BN film but an epitaxial transition from pure h-BN to nG-h-BN.

In order to gain further insight into the origin of the nG-h-BN X-ray photoelectron spectroscopy (XPS) was acquired on the pure h-BN and the nG-h-BN phase grown on Rh(111) (Figure 3). Apart from Rh the XPS survey taken on nG-h-BN shows only carbon, nitrogen, and boron as chemical components (see Supporting Information). The binding energy of the main peaks of N 1s and B 1s agree with the binding energies published for h-BN.[30] The B 1s shows a small component at lower binding energy besides the main peak (Figure 3c) which is probably due to some contaminations like BHx remaining from the borazine precursor. The C 1s peak for the nG-h-BN phase exhibits a binding energy of 284.5 eV, which is in line with the binding energy of sp2 carbon[31] and comparable to the C 1s peak observed for weakly coupled graphene on Rh(111).[32] Since transition metal carbides usually exhibit a binding energy below 284.0 eV we can exclude the formation of RhC at the interface.[33] Figure 3b also reveals that the C 1s peak area on the h-BN phase is much smaller than the one on nG-h-BN. Additionally, the C 1s peak of the pure h-BN phase is slightly shifted towards lower binding energies (284.2 eV) which might be due to better screening of the carbon dissolved in the Rh(111) compared to the carbon on top of the Rh(111). Thus, we conclude that this small carbon amount observed for the pure h-BN results from carbon dissolved in the subsurface region of the Rh, which should not have any influence on the properties of the pure h-BN. Furthermore, no additional shoulders at higher binding energy in the C 1s and N 1s spectra for nG-h-BN are visible. Such peaks at higher binding energies were reported for in-plane h-BN-G heterostructures due to the C–N bond.[34,35] In conclusion, our hypothesis that the nG-h-BN is created by graphene nanoflakes embedded between the h-BN wire sites and the Rh(111) is confirmed by the XPS measurements, which indicate sp2 hybridized carbon and no C–N bonds in the C 1s and N 1s spectra.

To understand the formation of the nG-h-BN phase, DFT calculations were carried out for the pure h-BN/Rh(111) structure and that with graphene nanoflakes of different sizes embedded between the Rh(111) surface and the h-BN layer (Figure 4, see Supporting Information for different sizes of the graphene nanoflakes). With about 2.2–2.4 Å, the h-BN pores have the shortest distance to the metal substrate, and thus have the highest interaction strength.[36] Therefore, modification of this area by intercalation of carbon atoms is not energetically favorable. Instead, a much weaker interaction strength is indicated for the wire areas (as defined in Figure 1a), since
there the height between N atoms and the metal substrate ranges from 3.89 to 4.00 Å. Therefore, the wire area is the most plausible position for intercalating carbon atoms. It is well known that the theoretically derived corrugation is strongly functional dependent,[37] and the value presented here is larger than recently determined by X-ray photoelectron diffraction[17] but the value which we found in our DFT calculations fits well with the one determined by Gubo et al.[38] Since we observed triangularly arranged defects in the STM measurements (see Figure 2a), which we attribute to the starting configuration of the nG-h-BN phase, we placed graphene nanoflakes with different numbers of carbon rings at the respective positions of the h-BN Moiré structure. The detailed adsorption geometry for graphene nanoflakes containing five carbon rings is depicted in Figure 4. In addition to a stronger corrugation of the h-BN sheet due to the carbon intercalation, reduced size of the pores was observed. We found that the lowest energy is obtained for carbon rings accumulated with their center on top of Rh atoms, in agreement with the formation of graphene on Rh(111).[19]

Figure 5 shows the comparison between experimental and simulated STM images of nG-h-BN/Rh(111) with one and five carbon rings intercalated. The simulated STM image with one carbon ring at each corner of the triangle fits well with the observed STM images of the trian-gularly arranged defects (Figure 5a,c,e). These defects, which are probably a precursor state of the nG-h-BN, appear as regular triangles with the corners exhibiting an increased apparent height. For the simulation with graphene nanoflakes consisting of five carbon rings, clear structures of triangular regions with high and low apparent height are found in the simulated STM image (Figure 5d). One can see that the structures of the bright and dark triangles, as well as the hexagonal shape of the pore observed in the experiments are well reproduced by the calculations for the intercalation of five carbon rings. In short, considering the experimental and theoretical results presented so far, the origin of nG-h-BN can be ascribed to intercalated carbon in the form of graphene nanoflakes between the Rh(111) surface and the h-BN layer at the wire sites.

The carbon intercalation also influences the electronic structure of the system. Distance to voltage spectra (dz/dV) were acquired to probe changes of field-emission resonances (FERs)[40] and of the interface states. Thereby changes in the energetic positions of unoccupied states were obtained to gain insight into the modification of the electronic structure.

A series of dz/dV spectra were acquired along a line across a set of three pores (h-BN) and analogous for two dark triangles, one bright triangle and one hexagon (nG-h-BN) (Figure 6a). For the pure h-BN phase, one can see an interface state around 2.5 V predominantly present at the pore region. Comparison of the dz/dV spectra of the pure h-BN pore to the hexagon of the nG-h-BN indicates that both exhibit the same interface states and FERs (Figure 6a,c). The 2nd order FERs are shifted to higher energies by about 0.5 eV for the nG-h-BN hexagons compared to the pure h-BN pores. This effect is likely caused by different tip shapes and thus variations of the effective electric field inside the junction that are more prominent for the higher-order FERs.[41]

It is clearly visible that there are electronic states in the nG-h-BN phase, which do not have an obvious counterpart in the pure h-BN. The state at approximately 2.8 V (labeled A in Figure 6b) for the dark triangle and that at 1.9 V (labeled B in Figure 6a) for the bright triangle are probably the modified interface state. As a result of the modifications at the h-BN/Rh(111) interface, the above-mentioned states are significantly shifted compared to the original interface state at 2.5 V. The state around 5 V (labeled C in Figure 6a,b) at the bright triangle is also an interface state since its position is independent of the tip geometry. This state is well resolved in the dI/dV maps (Figure 6c) and it is clearly visible that it has no counterpart in the pure h-BN. We thus conclude that the intercalation of carbon at the corners of the bright triangles strongly modifies....

Figure 4. a,b) Top and side views of the corrugated structure of h-BN/Rh(111). c,d) Top and side views of the corrugated structure of nG-h-BN/Rh(111) with graphene nanoflakes consisting of five carbon rings. The different heights of the B and N atoms are color-coded in the figure. The black diamond indicates the surface supercell used in the simulations. Color code: Rh: grey, C: black, B: dark blue to light blue, and N: red to yellow.
the electronic structure of the h-BN probably as a result of a modified hybridization and charge transfer between the substrate and the h-BN by the intercalated graphene nanoflakes, which is further confirmed by DFT calculations (vide infra). In contrast, the hexagons and pores show similar electronic structures, which further support our hypothesis that these areas remain unmodified.

To further identify the similarities and differences of electronic structures between the respective regions of Moiré patterns for h-BN and nG-h-BN we compare the experimental results to the calculated electronic density of states (DOS). In the following, we will concentrate on the DOS of the wire areas and the bright triangles of h-BN and nG-h-BN, respectively, since these are the regions that show the strongest differences in the dz/dV measurements displayed in Figure 6.

Figure 7 shows the DOS of the wire areas of h-BN/Rh(111) and that of the bright triangles of nG-h-BN/Rh(111) for five carbon rings. Here the gap of h-BN disappears in the regions of the bright triangles (Figure 7b) and there are new unoccupied states above the Fermi level. The additional state below the onset of the h-BN DOS above 2 eV might be related to the interface state observed at 1.9 eV in the dz/dV spectrum labeled A in Figure 6b. The high intensity above 4.5 eV might be related to the modified interface state observed at 5 V for the bright triangles (C in Figure 6b). The results described above suggest that there are graphene nanoflakes containing five or more carbon rings intercalated between the h-BN and the Rh(111), which leads to the observed changes in the DOS of the regions of the bright triangles in the nG-h-BN structure. This again supports our earlier findings that the experimental data can be well described by the intercalation of graphene nanoflakes consisting of five or more hexagonal carbon rings.

As an additional probe for the modified properties of nG-h-BN, we investigated whether it has altered active sites towards molecular adsorbates compared to h-BN. Since the adsorption of pentacene on h-BN was studied previously,[42] we performed a similar study of pentacene on nG-h-BN. An STM topography image of the resulting sample surface after adsorption of pentacene on nG-h-BN/Rh(111) is depicted in Figure 8a. The pentacene molecules appear as rod-like objects when imaged in the energy range of the highest occupied molecular orbital-lowest unoccupied molecular orbital (HOMO-LUMO) gap. In contrast to h-BN, for which the adsorption position of pentacene was defined by the dipole rings inside the h-BN pore,[43] the molecules are now exclusively found at the edges between the dark triangles and the hexagons in proximity to the dark wires of the nG-h-BN (Figure 8b). They adhere in such a way, that the long axis of the molecule is aligned in parallel to one of the triangle’s edges. Similarly, to the case of pentacene adsorbed on pure h-BN, the molecules here are efficiently decoupled from the substrate, which can be seen by the dz/dV map taken at –2.1 V imaging the HOMO of the pentacene molecule (inset in Figure 8b).

As in the experiments, our calculations also indicate that the pentacene molecules are oriented with their long axis along the dark triangle (Figure 8d). However, the calculated adsorption position is shifted slightly towards the center of the dark hexagon in contrast to the STM images (Figure 8c). Earlier calculations showed that the adsorption energy landscape of organic molecules on h-BN is rather shallow and depends on the exact functional used, which might explain the discrepancy between the adsorption position determined by STM and by DFT.[44]

The altered electronic structure of nG-h-BN/Rh(111) is also reflected in the charge density differences between nG-h-BN/Rh(111) and h-BN/Rh(111) as presented in Figure 9. In the presence of the graphene nanoflakes, there is charge excess over bright triangles while on dark triangles there is a charge loss. We thus conclude that the growth of graphene nanoflakes strongly affects the electronic as well as the chemical structure of h-BN/Rh(111).

3. Conclusion

We prepared graphene nanoflakes by the intercalation of carbon between h-BN and the Rh(111) substrate by means
of a segregation growth method. With the combined study of high-resolution STM and STS together with XPS measurements and DFT calculations, we showed that the structure originates from small domains of $sp^2$-carbon.

**Figure 6.** Electronic structure of $h$-BN and $nG$-$h$-BN: a) Line profiles of the energetic position of the FERs on $h$-BN (left) and $nG$-$h$-BN (right). The corresponding spatial positions are indicated in the STM topographies (red dashed line). Dashed black line: Position of the 1st FER ($h$-BN). Dashed white line: Position of the interface state ($h$-BN). Dashed white ovals: New states at the positions of the dark and bright triangle ($nG$-$h$-BN); (settings for the STM images: $-3.0$ V, 4 pA for $h$-BN, $-2.0$ V, 10 pA for $nG$-$h$-BN); b) $dz/dV$ spectrum acquired on the position of the bright triangle of $nG$-$h$-BN ($I = 50$ pA). The positions of the individual peaks are indicated; c) Spatial mapping of the interface states at 2.0 (State A), 2.5 (Interface State), 3.0 (State B), 4.5 (1st order FER of the $h$-BN wires), and 5.0 V (State C) by $dI/dV$ maps ($I = 500$ pA) at a region where both phases co-exist. The area of the $h$-BN region is marked by the blue contour. The blue hexagons and circles mark the hexagon and the pore of $nG$-$h$-BN and $h$-BN, respectively. The corresponding STM topography of the area utilized for this measurement is depicted in the upper left image.

**Figure 7.** DOS of N and B atoms of the wire in $h$-BN/Rh(111) (purple line) and of the bright triangle region (blue shadowed area) of $nG$-$h$-BN/Rh(111) calculated for five carbon rings. Right: The zoom-in of the states of the bright triangle near the Fermi level.
nanoflakes forming at specific registries, at the position of the highest distance between h-BN and Rh(111) substrate. The altered adsorption positions for organic molecules represent a change of the local reactivity of the nG-h-BN phase compared to the original h-BN surface structure. In our study, the preparation of the graphene nanoflakes/h-BN heterostacks was possible in a one-step process, which is most likely scalable for wafer-size production and thus a promising route for the preparation of similar heterostructures.

Figure 8. Pentacene adsorption on nG-h-BN: a) Overview STM image showing the nG-h-BN Moiré structure and the pentacene molecules appearing as rod-like protrusion; b) Close-up view: the position of the pentacene molecules at the edges between the dark triangle and hexagon is indicated (scanning parameters for both images: \( U = -1.0 \, \text{V}, I = 100 \, \text{pA} \)); The inset shows a \( dI/dV \) map of the HOMO of a pentacene molecule (\( U = -2.1 \, \text{V}, I = 100 \, \text{pA} \)); c) Simulated structure of pentacene on nG-h-BN/Rh(111) with five carbon rings: color code is the same as in Figure 4. d) Simulated STM image (\( U = -1.0 \, \text{V} \)) for the structure shown in (c).

Figure 9. a) Top and b,c) side views of charge density difference of nG-h-BN with five carbon rings with respect to h-BN/Rh(111). The charge density at (a) is cut at 1 Å above the bright triangles. Charge difference cut in directions of the red line (b) and the blue line (c). The dark and bright areas show charge loss and excess, respectively; right: scale bar of the charge difference, the units are in e Bohr\(^{-3} \).

4. Experimental Section

**Experimental Details:** All experiments were performed under ultra-high vacuum (UHV) conditions. Initial UHV cleaning of the Rh(111) single crystal surface was performed by repetitive cycles of Ar\(^{+} \) bombardment and subsequent heating to 800 °C for 5 min. Since Rh crystals provide native bulk impurities (mainly carbon and sulfur) which upon annealing diffuse to the surface, the crystal was heated to 830 °C under continuous Ar\(^{+} \) ion bombardment. In order to decrease the carbon depletion layer thickness, the samples were sputtered cold prior to nG-h-BN growth. For both phases, h-BN was grown in a CVD process at a substrate temperature of 800 °C with borazine as a precursor. A total dosage of 110 L was necessary for full coverage of the Rh(111) surface with a monolayer of h-BN or nG-h-BN. The liquid borazine was cleaned in freeze-pump-thaw cycles removing volatile contaminants using liquid nitrogen prior to the exposure. Pentacene was deposited in situ using organic molecular beam epitaxy.

The samples were prepared in a homebuilt STM under UHV conditions at 5 K using tungsten tips. To gain insight into the structure of the sample surface, the topography was investigated in constant current mode, unless otherwise stated. Furthermore, a high structural resolution was achieved by operating the STM in point contact mode at a conductance of 9 × 10\(^{-6} \, \text{S} \). This allowed for imaging of individual atomic bonds. WSxM was used to analyze the STM images.\(^{[43]} \) To probe the electronic properties of the films, STS experiments and spatial mapping of the differential conductance using a lock-in technique were employed (typical parameters: modulation frequency: 832 Hz, amplitude: 50 mV (peak-to-peak)).

XPS, ultra-violet photoelectron spectroscopy (UPS), and low-energy electron diffraction (LEED) measurements were performed in a separate multi-chamber UHV system at room temperature. The samples were prepared in situ similar to the recipe described above. High-resolution XPS data were acquired with a Kratos Axis Ultra system used together with a monochromatized Al K\(_{α}\) X-ray source. UPS measurements were acquired with a monochromatized HeI source (21.2 eV) and a SPECS 150 hemispherical analyzer under normal emission with an acceptance angle of ±9°. The preparation chamber contains a LEED optics (SPECS ERLEED 1000-A), which was used to obtain the LEED images.

Theoretical Details: DFT calculations\(^{[46]} \) were performed employing the projector-augmented wave (PAW),\(^{[47]} \) plane-wave basis set, and the supercell method as implemented in the Vienna Ab-initio Simulation Package (VASP).\(^{[48]} \) The exchange-correlation interaction of electrons was described by the generalized gradient approximation (GGA) in the form of the Perdew–Burke–Ernzerhoff (PBE) functional.\(^{[49]} \) The cutoff for the kinetic energy of the plane-wave expansion was set to 500 eV.
To include dispersion correction the DFT-D3 correction was used. In the calculations, the supercell of h-BN/Rh(111) was used, in which the periodicity of the pore was ≈3.2 nm, close to the experimental values of 3.14 ± 0.1 nm and those in the literature. The supercell consists of a three-layer, 12 × 12, Rh(111) slab constructed with an optimized lattice parameter of 3.79 Å and a 13 × 13 monolayer of h-BN with a bond length of 1.46 Å and a vacuum of 20 Å to separate the slab and its normal periodic images. The total number of atoms in the unit cell varies between 601 for the h-BN/Rh(111) system and 658 atoms for the nG-h-BN/Rh(111) system with five carbon rings at the positions of the bright triangles. The Brillouin Zone was sampled with one point at the zone center. For simulation of hexagonal carbon rings intercalated underneath the h-BN wire areas (two such areas exist, one closer to the Rh(111) surface than the other), the rings were placed under every other wire area, selecting the one in which h-BN was further away from the Rh(111) substrate. Furthermore, these carbon rings (1–5) formed a triangle, that is, the 1–5 membered rings exist at the corners of a triangle. To find the lowest energy configuration of the carbon rings on top of the Rh(111) substrate, the systems were simulated with the rings at all high symmetry points such that either the center of these rings was placed on the FCC, HCP, TOP, or Bridge site or one of the carbon atoms in the ring was placed exactly on these high symmetry points. All structures were relaxed until all components of the force acting on each atom were smaller than 0.01 eV Å\(^{-1}\). All atoms were allowed to relax in all directions except those in the bottom layer of Rh(111), which was held fixed in all calculations. For simulations of STM images and calculations of DOS, the Brillouin Zone was sampled by a 3 × 3 × 1 k-point mesh.

Simulated topological STM images for bias voltages U were approximated to be the 10\(^{-3}\) e Å\(^{-1}\) isosurface of the local density of states (LDOS) contributed from all states that lie between \(E_F\) and \(E_F + 1\) eV, where \(E_F\) is the Fermi level. To make the simulated STM images comparable to the experimental ones, a Gaussian filter with \(\sigma = 0.5\) Å was used. The charge density difference was obtained using:
\[
\Delta \rho = \rho_{nG-h-BN} - \rho_{h-BN}, \quad \text{with} \quad \rho_{nG-h-BN} \quad \text{and} \quad \rho_{h-BN} \quad \text{as the total charges densities of the nG-h-BN and h-BN on the Rh(111) substrate, respectively.}
\]

To find the adsorption position of pentacene on both nG-h-BN/Rh(111) and h-BN/Rh(111), all obviously possible starting positions were considered and the systems were relaxed until the force on each atom in all the directions was smaller than 0.02 eV Å\(^{-1}\). Similar to the relaxation setup of clean surfaces, all atoms were allowed to move except for those in the bottom layer of Rh(111) which were kept fixed during the relaxation.

Supporting Information

Supporting Information is available from the Wiley Online Library or from the author.

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Conflict of Interest

The authors declare no conflict of interest.

Data Availability Statement

The data that support the findings of this study are available from the corresponding author upon reasonable request.

Keywords

2D heterostructures, density functional theory, hexagonal boron nitride, scanning tunneling microscopy and spectroscopy

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