The Reactivity of Hexagonal Boron Nitride Defects

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The properties of epitaxially grown 2D materials, such as hexagonal boron nitride (hBN) and graphene, depend on the growth mechanism and defects in the epitaxial layer. In our study, we employ Density Functional Theory (DFT) calculations to examine the epitaxial growth of hBN on a Ru(0001) surface; we have developed a detailed understanding of the formation of hBN from borazine. Our results predict the formation of a (3 × 3) meta-stable structure, consistent with results from helium atom scattering experiments.[1] Building on this finding, we have determined the behaviour of an isolated borazine molecule on a Ru(0001) surface and have investigated its polymerisation. Then we determined a detailed hexagonal boron nitride growth mechanism on Ru(0001). Our findings have implications for CVD processes, the creation of defect sites and the design of new nanomaterials based on exploiting the growth phases of hBN.

We have also investigated the effect of defects on the catalytic activities of hBN. The many advantages of hBN for heterogeneous catalysis include high surface area, thermal stability, and durability. Furthermore, hBN is more sustainable than the ubiquitously employed precious and transition metal-based catalysts. Through DFT simulations, we have explored metal-free hBN as a valid alternative to precious metal catalysts for producing H_2 via the reaction of ammonia with a surface boron and nitrogen divacancy (V_{BN}), achieving a decomposition barrier of 0.52 eV. For comparison, the reaction of ammonia with epitaxially grown hBN on a Ru(0001) substrate was investigated, and we observed similar NH_3 decomposition energy barriers (0.61 eV) but a much more facile H_2 desorption barrier (0.69 eV vs 5.89 eV).[2] We have continued to investigate how a hydrated vacancy can participate in the hydrogenation of NO_x to H_2O. Through completing this work, we hope to discover sustainable alternative catalysts.

Acknowledgments

Please acknowledge here funding sources if necessary.

[1] A. Ruckhofer, et.al., "Evolution of ordered nanoporous phases during h-BN growth: Controlling the route from gas-phase precursor to 2D material by in-situ monitoring", Nanoscale Horizons, 7. 1388–1396. (2022)

[2] A. Payne, et.al., "Dehydrogenation of ammonia on free-standing and epitaxial hexagonal boron nitride", Phys. Chem. Chem. Phys, 24. 20426–20436 (2022).