The University of Texas Rio Grande Valley
Center for Multidisciplinary Research Excellence in Cyber-Physical Infrastructure Systems (MECIS)

Development of Boron Nitride-Based Composites for Enhanced Gas Sensing Applications

National Science Foundation
NSF Award No. 2112650

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Abstract

We present a combined computational and experimental work on defect-modified hexagonal boron nitride(h-BN) monolayers for CO gas detection applications. Using Density Functional Theory (DFT), we calculated the electronic and optical properties of defect h-BN to predict its response to CO adsorption. CO induces distortions on the BN lattice, the emergence of new states under the conduction band, and an alteration in the imaginary part of the dielectric function. Silver-doped BN nanoparticles were synthesized and characterized using structural and morphological analysis methods. Silver-doped boron nitride nanoparticles exhibit a promising potential to serve as gas sensor material.

Introduction & Background

Hexagonal boron nitride (h-BN) is a versatile material known for its excellent thermal stability, not being chemically reactive, and layered structure. BN is non-conductive, but doping BN improves conductivity and allows usage as gas sensing material.
Doping BN with metals, particularly gold, platinum, and silver, introduces new functionalities, especially in the area of gas sensing. Doping enables improved electronic and catalytic properties, enhancing its sensitivity and selectivity to target gases, such as CO.
The present work investigates the development of doped BN nanoparticles that are received from autoclave reaction in the system BN-$AgNO_3$-PVP, which produces nanoparticles for gas sensing applications, aiming to leverage the high surface area of h-BN and the improved conductivity due to doping with silver, while using PVP as reducing agent to receive silver from the nitrate.

Methodology

To synthesize silver doped BN, boron nitride (BN) was combined with silver nitrate ($AgNO_3$) and polyvinylpyrrolidone (PVP), BN and $AgNO_3$ were combined in a 1:1 molar ratio with 0.01 mmol of PVP. This mixture was placed in a 50 mL Teflon-lined autoclave containing 30 mL of N,N-dimethylformamide (DMF). The autoclave was then heated to 160°C for 8 hours and left to cool to room temperature. The resulting product was washed sequentially three times with deionized water and ethanol. Lastly, material was dried in an oven for 12 hours at 80 °C.
DFT electronic structure calculations, optimal geometries, and the dielectric functions were obtained for optimized defect *h*-BN monolayer with/without adsorbed CO using the periodic code Vienna Ab initio Simulation Package (VASP). The projector augmented-wave (PAW) pseudopotentials were used. The Kohn–Sham equations are solved using the generalized gradient approximation (GGA) under the Perdew–Burke–Ernzerhof (PBE) functional form.

Data and Results

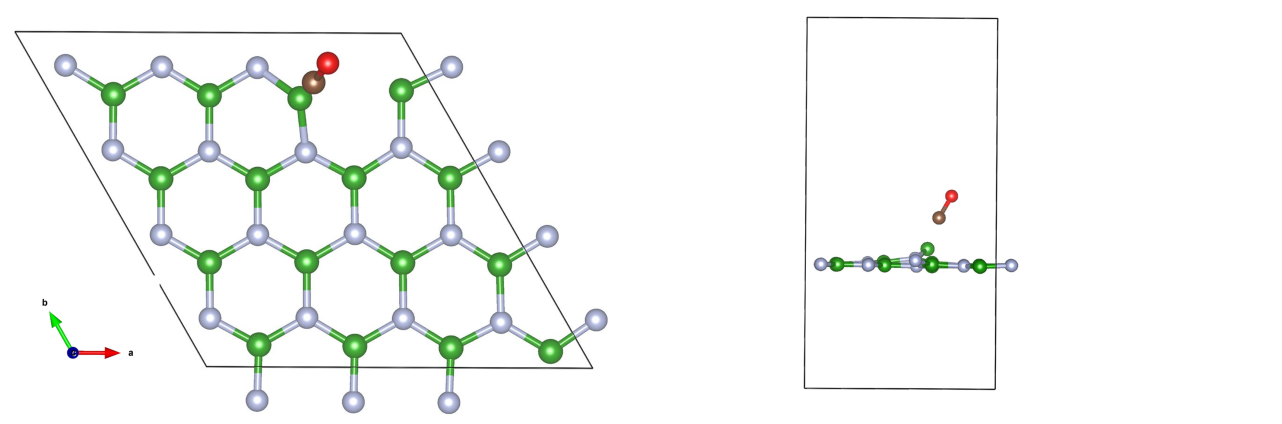

Figure 1-The top view of the DFT optimized defect h-BN monolayer with the adsorbed CO as a 4×4×1 supercell (b) its side view. Atoms are colored as follows: B, green; N, gray; C, brown; O, red. The thin black lines denote the supercell boundaries.

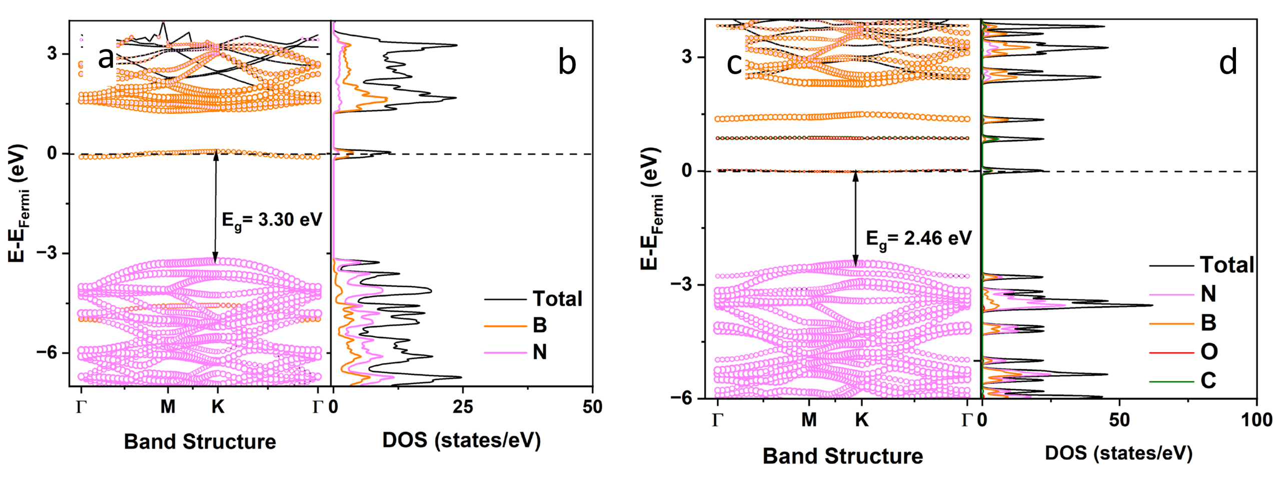

Figure 2 - (a) Electronic band structure for defect *h*-BN and (b) its densities-of-states (DOS), (c) band structure for defect *h*-BN with adsorbed CO, and (d) its DOS.

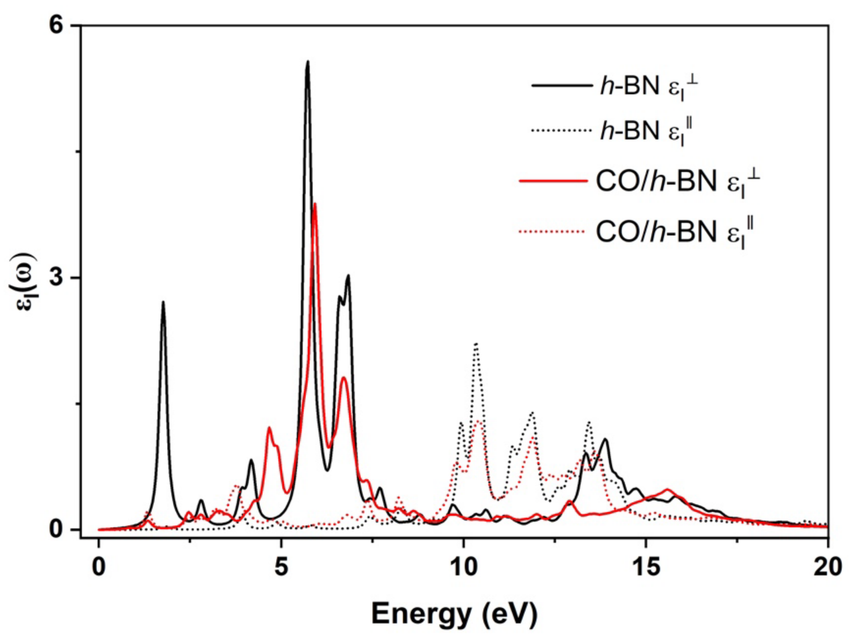

Figure 3 – The imaginary part of the dielectric function for the defect BN with and without the absorbed CO. The perpendicular and the parallel to the c-axis components are shown.

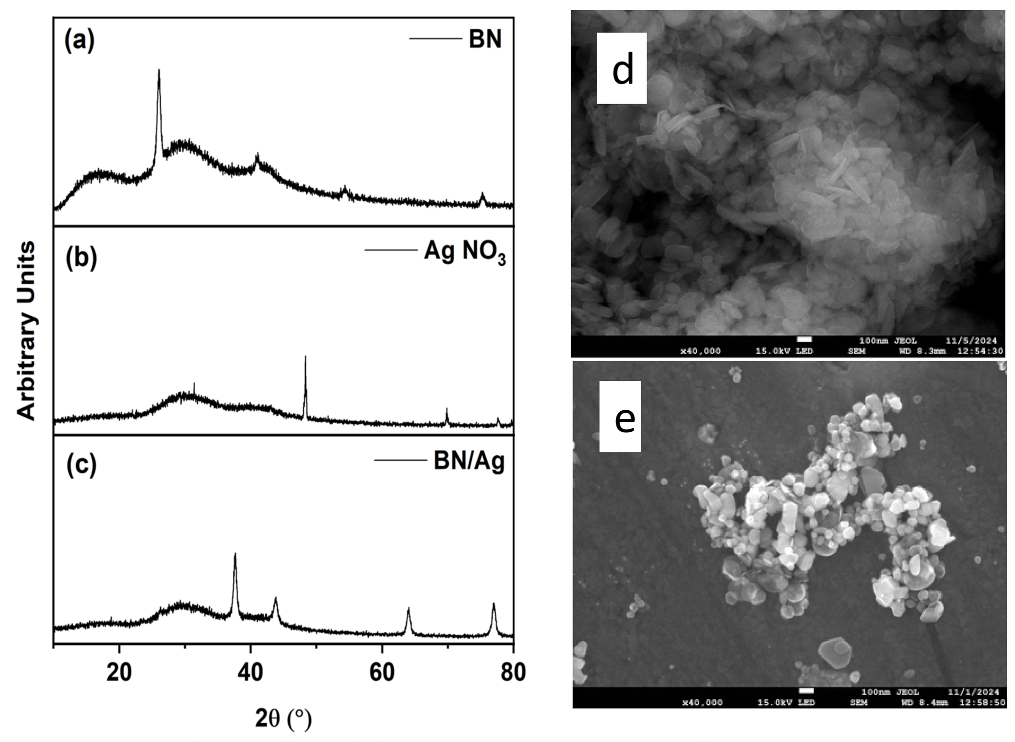

Figure 4- (a,b,c) XRD pattern obtained for nanosized BN, $AgNO_3$, BN-$AgNO_3$-PVP, (d) SEM of precursor BN, (e) silver doped BN nanoparticles

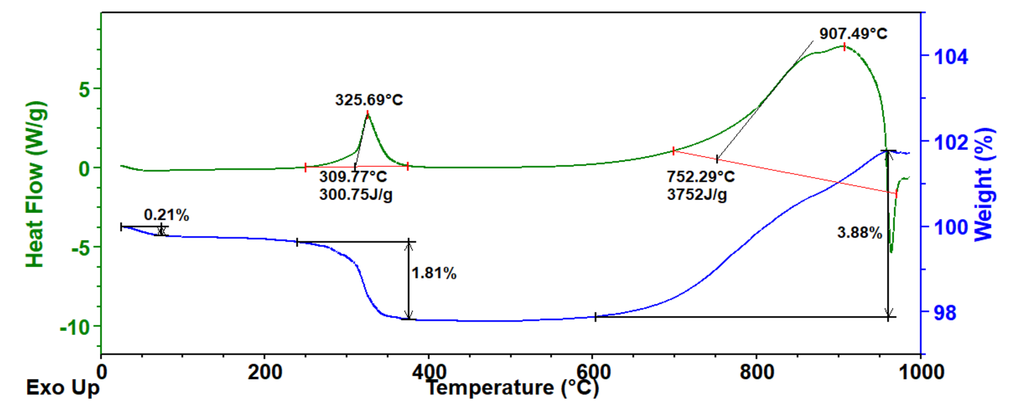

Figure 5 – DSC/TGA analysis for BN-$AgNO_3$ –PVP system.

Conclusions & Future Work

We demonstrate the potential of defect-engineered hexagonal boron nitride (h-BN) for CO gas detection, with calculations illustrating how CO interactions at vacancies within the BN monolayer distort the lattice structure and significantly influence the material's optical and electronic properties. The practical application of BN as a gas sensor is ensured by doping it with silver, which improves the electrical properties. The autoclave method enabling synthesis of silver doped BN is nanoparticles. These nanoparticles form homogeneous layers suitable for four-point sheet resistance measurements, highlighting their potential in gas sensor applications.

Acknowledgments

The authors would like to acknowledge funding provided by the National Science Foundation CREST Center for Multidisciplinary Research Excellence in (NSF Award No. 2112650).

References

[[1] A. Sultan, F. Mohammad, "Chemical sensing, thermal stability,electrochemistry and electrical conductivity of silver nanoparticles decorated and polypyrrole enwrapped boron nitride nanocomposite" ,*Polymer,* vol.113, 221-232 (11 pages), 2017