η⁶ Organometallic Hexagonal Boron Nitride: Functionalization and Properties

Kartikey Sharma
Songwei Che, Naveen Dandu, Anh Ngo and Vikas Berry*
University of Illinois at Chicago, 929 W Taylor St., IL 60607, United States
ksharm40@uic.edu, vikasb@uic.edu

Abstract

Hexagonal boron nitride (h-BN), renowned for its formidable attributes—tensile strength (~100 GPa), wide bandgap (~6 eV), high thermal conductivity (227-280 $W.m^{-1}.K^{-1}$), and chemical stability—poses a challenge in functionalization due to its electronegativity variance between boron and nitrogen.[1,2] In a breakthrough, we present unprecedented organometallic functionalization via chromium carbonyl vapor exposure. This novel approach forms a pristine η6 bonding that preserves lattice planarity and interconnectivity between B- and N-centers, with the metal engaging each hBN ring. Computational analysis validates spontaneous surface reaction (ΔG = -35.50 kcal/mol). Further, carbonyl groups seed silver nanoparticle growth, culminating in a conductive layer atop hBN. Fourier transform IR spectroscopy, Raman Spectroscopy and X-Ray photoelectron spectroscopic techniques reveals the molecular reaction mechanism involved in this functionalization. This non-destructive, chemically versatile functionalization ushers in a new era in multifunctional coatings, harnessing hBN's thermal and structural prowess across diverse applications.

References

[1] Golberg, D. *et al.* Boron nitride nanotubes and nanosheets. *ACS Nano* **4**, 2010, 2979–2993.

[2] Petrone, N., Cui, X., Hone, J., Chari, T. & Shepard, K. Flexible 2D FETs using hBN dielectrics. *Technical Digest - International Electron Devices Meeting, IEDM*, 2015, 19.8.1-19.8.4

Figures

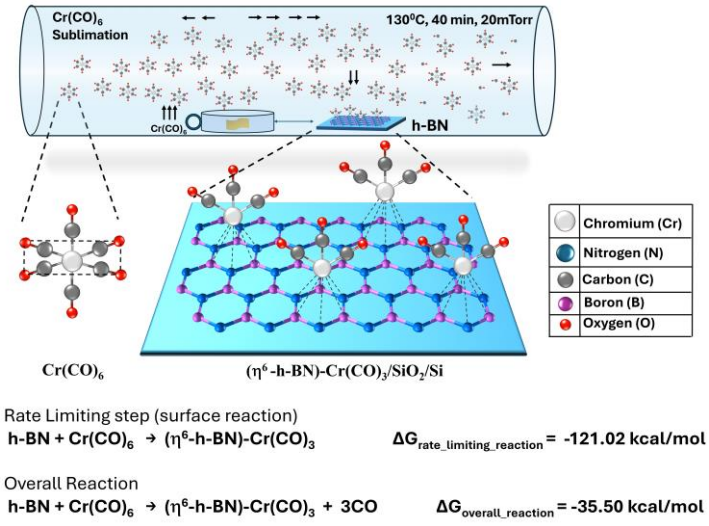

Figure 1: Schematics of h-BN functionalization with chromium hexacarbonyl ($Cr(CO)_6$) via chemical vapor deposition (CVD) in 1inch quartz tube.