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Research Articles

# Boron carbide biodevices for disease-specific biomarker detection: a theoretical study

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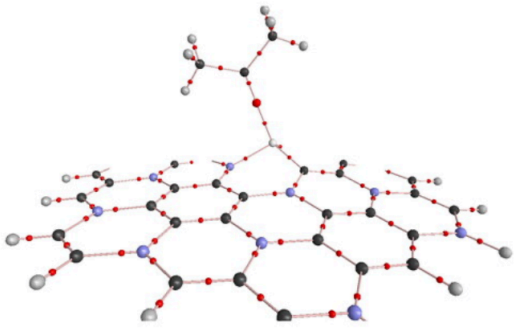
## Abstract

An effective approach for early diagnosis of lung cancer involves detecting its biomarkers in the patient's exhaled breath. Acetone was identified as a vital biomarker, showing significant elevation in lung cancer. Two-dimensional boron carbide materials offer benefits such as resistance to high temperatures, stability, and excellent sensitivity toward toxic gas molecules. Here, we explore acetone adsorption on the pristine and transition metal (TM)-doped (Sc, Ti, V, Cr, and Mn) boron carbide monolayers (BCMs) with density functional theory calculations. Our results revealed that the V-, Cr-, and Mn-doped BCM show larger adsorption energy values as compared to the pristine BCM surface. The change of band gap energy of surfaces after acetone adsorption is obtained between 55 and 275%. The work function variation of studied monolayers upon acetone adsorption has been also investigated and results show that V-, Cr-, and Mn-doped BCM systems are sensitive to acetone gas molecules. This work suggests that BCM-based layers can be used as a biosensor to identify VOC biomarkers such as acetone.



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**Keywords:**

Volatile organic compounds | biomarkers | acetone | 2D materials | density functional theory