Investigation and Design of Two-Dimensional Nanomaterial Biosensors for Breath-Based COVID-19 Detection Using Density Functional Theory

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Current COVID-19 testing is invasive and requires certain equipment, making screening difficult without such devices. Furthermore, when testing can be expedited, it often brings with it a substantial false-negative rate. There is urgent need for a 2D nanomaterial to be a highly sensitive, portable, low-cost biomarker sensor. Three COVID-19 biomarkers (Ethyl Butyrate, Methanol, and Heptanal) have been identified in recent research. Computational approaches have facilitated the transition from theoretical work into direct applications, and are implemented here. This is the first report in which the interaction between hexagonal Boron Carbide and selected COVID-19 biomarkers have been studied using a first-principles approach based on density functional theory. In this research, four dopants were chosen for their electron structure to modify BC3: Al, Si, P, and As. The BC3 variants were evaluated on biomarker adsorption strength and sensitivity (change in electrical conductivity upon adsorption). Pure BC3 monolayers were found to be ineffective due to low adsorption strength and sensitivity, making BC3 a poor biosensor for COVID-19 biomarkers. However, Al- and Si-doped BC3 were found to be effective in forming a strong interaction and demonstrated high sensitivity. Moreover, Al-doped BC3 was calculated to have the shortest recovery time, making it a promising 2D nanomaterial biosensor for COVID-19. Based on the findings in this research, a novel multi-biomarker COVID-19 screening device is proposed by fully utilizing and profiling the interaction properties between BC3-based 2D nanomaterials and the selected biomarkers. These findings will facilitate the development of a 2D-nanomaterial based COVID-19 biosensor which can substantially address issues in current testing.

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