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Evaluation of the Feasibility of Phosphorene for Electronic DNA Sequencing Using DFT Calculations BENJAMIN TAYO, University of Central Oklahoma, SANJIV JHA, East Central University — Electronic DNA sequencing using two-dimensional (2D) materials such as graphene has recently emerged as the next-generation of DNA sequencing technology. Owing to its commercial availability and remarkable physical and conductive properties, graphene has been widely investigated for DNA sequencing by several theoretical and experimental groups. However, due to the hydrophobic nature of graphene, DNA bases to stick to its surface via strong pi−pi interactions, reducing translocation speed and increasing error rates. To circumvent this challenge, the scientific community has turned its attention to other 2D materials beyond graphene. One such material is phosphorene. We performed first-principle computational studies using density functional theory (DFT) to evaluate the ability of phosphorene to distinguish individual DNA bases using two detection principles, namely, nanopore and nanoribbon modalities. We observe that binding energies of DNA bases are lower in phosphorene compared to graphene. The energy gap modulations due to interaction with DNA bases are very significant in phosphorene compared to graphene. Our studies show that phosphorene is superior to graphene, and hence a promising alternative for electronic DNA sequencing.

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