Multidisciplinary Research on Graphene Biosensors

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Abstract

Applications of graphene for the design of electrical biosensors face certain limitations that could be addressed by applying a multidisciplinary approach to describe the complexity of nanoscale systems. The sensitivity of functionalized graphene structures for virus detection is reduced due to the short Debye length in typical solutions like the phosphate-buffered saline (PBS) solution. Seemingly unrelated studies in ionic solutions and electrolytes analyse the Debye length from a different point of view. Graphene planar surfaces are seldom implemented in two-plate capacitor settings for bioresearch. There are some studies of the Debye length in parallel plate capacitors [1] that could be extended to graphene plates for a better understanding of long-range Coulomb interactions. An increase of the molarity in ionic liquid solutions follows to an increase of the electrostatic screening length after a certain threshold [2]. Efforts to design biosensors beyond the Debye length limit in high ionic strength solutions are reported in [3]. This topic becomes increasingly important as the research community puts a great effort to cope with the coronavirus disease 2019 (CoViD-19) pandemic. There are various technologies involving graphene that take part in the fight against CoViD-19 [4]. In order to reach a Debye length comparable with the expected size of a chosen antibody on the graphene surface (provided to bind the S1 subunit protein from COVID-19), a diluted 0.01xPBS solution of 1.6-Mm molarity and 7-nm Debye length is utilized [5]. Note that the size of the coronavirus is much larger than both the binding segment in a single S-protein spike and the Debye length. This makes it challenging to estimate statistically the number of binding events and the resultant electrical effect in the graphene sensor configuration. Further evaluation of the Debye length in ionic solutions between functionalised graphene plates with the application of ac voltage at different amplitudes and frequencies is the next logical step in understanding the optimal biosensor sensitivity. The optimal molarity for a given design is also to be determined. Since such empirical experiments could be costly and time consuming, the use of computational experiments and computer simulations with the involvement of researchers from diverse fields, not only in materials science and physical chemistry, but also in computer science and artificial intelligence (AI), is an essential part of the multidisciplinary research on graphene-based applications. Therefore, there is a specific niche in biosensing beyond the Debye screening. Said niche also involves graphene plasmonics. The unique properties of the two-dimensional graphene lattice result in the superior sensitivity of graphene biosensors. While new empirical works on testing various hybrid graphene sensors are reported daily, related theoretical and computational studies are less frequent. This could be attributed to the complexity arising from evaluating combinations of biological, physicochemical, and condensed matter phenomena. It should be noted that most experiments for commercial biosensors are performed at room temperature. The Debye length depends on the temperature as by definition it describes large thermodynamic systems of mobile charges. The thermal conductivity of graphene, graphene oxide (GO), and other graphene materials depends on the biosensing functionalization of its surface. Thus thermal conductivity is an additional useful characteristic for the design of graphene biosensors. In summary, this contribution provides a description of some proposed modifications for biosensor design and key points for performing computational studies involving the Debye length in ionic solutions at the surface of graphene structures.

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