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Theoretical Prophecies for Gas Detection by Layered Nanomaterials: An Outlook from Density Functional Theory

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Abstract

Layered two dimensional nanomaterials consisting of delocalized charged constituents in general, such as graphene and other allied carbon nanomaterials, transition metal dichalcogenides, MXene, etc., especially those which are semiconductor in nature, though possessing a tunable bandgap, are of particular interest to scientists engaged in exploring new materials for improved energy storge, conversion, gas detection, carbon capture etc. Conduction of physical experiment for such survey is of utmost importance before accepting a specific substance to be fit for any particular usage, ca. gas detection. It is necessary for the substance to qualify for satisfactory level of sensitivity, selectivity, response time, recovery time etc. for the intended gas. Yet, the lower bound of length scale for such experiment is always limited to certain minimum dimension which is unable to explain the actual mechanism behind the gas sensing phenomenon from electronic interaction point of view. One promising resolution to this issue is density functional theory (DFT) calculation to theoretically simulate the sensing phenomenon. Adaptation of such theoretical approach is beneficial in predicting feasibility of gas detection for any detector-analyte couple through calculation of binding energy, and explaining the inherent mechanism by orbital interaction analysis, charge transfer calculation etc. Such strategy is also capable of reducing the cost of expensive physical experimentation so that pragmatic researchers gather a first-hand idea about worth of involving huge capital towards fabricating any particular gas sensor. The current work is to present a precise concept about DFT calculations for prediction of layered nanomaterials as gas detectors.

Keywords: Layered Nanomaterials; Density Functional Theory; Gas Detection

Introduction

Gas sensor, as a vital expedient to perceive harmful gases, offers a vibrant course to watch the density and ecological info of gas in view of assuring the protection of ecology [1]. The gas-detection course comprises very feeble communications that are tough to sense in practice. Computations may deliver significant perception regarding the detection method, e.g., probable adsorption conformations, favored adsorption places, adsorption energy, charge transport, alterations in optical and electronic attributes, and diverse styles to improve adsorption which may partake a dynamic part in the progress and manufacture of effectual gas and biomolecule detectors [2]. 2D nanostructured resources, counting graphene-based structures [3], phosphorene [4], silicene [5], germanene [6], metal oxides [7], transition metal dichalcogenides [8], MXenes [9], binary oxides [10] etc. exhibit great gas-detection capability. The sensing mechanism of these 2D nanostructures are mostly electrochemical [11] in nature, i.e. chemiresistive, and charge transfer between host and analyte is the most important phenomenon behind the gas detection course. The efficacy of gas sensing for a particular layered nanomaterial depends on a host of vital characteristics such as the number of atomic layers, presence or absence of defects/dopants, the conductivity of the host etc [12]. The graphene-analogous nanosheets bid prospects to tailor them by means of surface functionalization, introduction of decorating substance or defects and formation of hybrid structure by combination with another material with varied constituents. Experiments are necessary to test competence of a gas sensor in terms of sensitivity, selectivity, specificity, response and recovery time etc [13]. However, finding the actual knowhow behind the sensing mechanism in terms of charge transfer in atomic scale is beyond the current capability of practical investigation, though

such information is quite necessary in order to design and develop cost effective gas detectors [14].

The outcomes forecast by hypothetical replications may corroborate well with the pragmatic quantities and offer meaningful thoughts for the associated detection mechanism. With the arrival of high-speed, huge-memory supercomputers, widespread electronic structure reproductions are nowadays pretty viable, and the calculation means and courses are improving every now and then [15]. Numerous renowned procedures for quantum calculations are braced by several nifty and widespread codes, both marketable and free [16]. Yet there are many contests for conjectural calculations: Detection parameters are quite complex to the selection of the replication inputs [17]. Thus, one has to be much cautious concerning the simulation actions and inferring the consequences. The basis of electronic structure simulations originates since the advancement and birth of quantum theory in the first part of last century [18]. Quantum theory not just provided an innovative intuition in consideration of physics but introduced accuracy and forecasting ability as well. The applicability of quantum mechanics is unlimited, whether it is in basic or functional twigs of science. Most significantly, a real-world course or scheme can be displayed using the equations of quantum mechanics [19]. Though, equations such as the Schrodinger equation may not be answered rationally excepting for some modest arrangements which are for the majority, extraneous for their minor gauges. Solving such an equation needs urbane numerical methods. These quantum mechanical approaches are inimitable in the sagacity that replicating system does not necessitate any experiential prototype or fitting parameters since they are first principle or ab initio in form [20]. In other words, such approaches do not need any erstwhile data from trials and may be utilized to investigate any prearranged scheme. Moreover, electronic structure simulations permit investigators to compute physical properties that may not be quantified straight or are unreachable for the pragmatists such as the binding energy of the atom or a molecule in a scheme. Such approaches can be incorporated in discovering novel compounds that can have a specific attribute and may be compared to current ones saving both experimental capitals and time. Numerous attributes of such supposed compounds can be foretold before turning it informal for the investigator while probing for a specific property. Hence, in general, simulations of materials deliver another stage of thought that may not be achievable since experiment.

Density Functional Theory (DFT) was recognized in 1964 with the two propositions hypothesized by Hohenberg and Kohn [21], followed by an array of equations developed by Kohn and Sham [22]. The cause DFT is well-thought-out as a foremost revolution in computational physics is for its correctness and viability. This turn DFT superior to other quantum chemistry methods e. g., the Hartree-Fock (HF) method [23] based on many-body wave function as the central capricious of the scheme. DFT on the other hand, considers the electron density. The key to notable accomplishment in DFT is the selection of appropriate approximations to the Exchange-Correlation Functional [24]. Yet, in order to refine the obtained outcome, many times it becomes necessary to incorporate suitable corrections such as hybrid functionals, dispersion force etc [25]. A few parameters are very significant for gaining rationally precise outcomes. These parameters may also be property reliant as the convergence of the property may depend on somehow completely diverse stricture standards. For instance, the energy cutoff (Ecut) is a vital constraint to attain correct magnitudes for the ground-state characteristics. Again, another imperative parameter for a precise DFT calculation is the k-point sampling. Unlike the Ecut, selecting an appropriate grid to model the Brillouin Zone is seldom a modest chore, and occasionally lower values for sampling may be more suitable than those at higher value.

The gas-detection knowhow in graphene and graphene-related layered inorganic analogs is founded on the charge transfer course where the sensing resource performs as charge donor or acceptor. This charge transport course alters the resistance of the detector substance which aids in sensing the gases. During the desorption procedure, the resistance of the detecting stuff yields to its original stage. Theoretical replication of 2D sensing materials is much valuable as it may impart thorough understanding about charge transportation, bonding, and orbital interactions which are tough to obtain by experiments. It may also investigate the detection machinery and sensing presentation of numerous resources to plan suitable sensor for the experimentalist to develop. Even though there are a number of ab-initio calculation approaches, e.g., DFT [21-22], Hartree-Fock [23], quantum Monte Carlo [26], coupled cluster [27], multireference configuration interaction [28], etc., the furthermost extensively used method is the first-principles calculation founded on DFT simulations since it rationally and proficiently defines the weak interaction between adsorbates and sensing resources. The outcomes foretold by DFT simulations may back pragmatic findings and offer theoretical insight on the mechanism of gas detection. Numerous mature marketable or free quantum software packages are available for carrying out electronic structure simulations in a convenient way. The greatest prevalent and vastly used such packages are VASP [29], SIESTA [30], Quantum Espresso [31], Abinit [32], etc. Interested readers may refer to a few recently published references [33-37] as examples for obtaining actual feel about the involved tasks usually done for theoretically simulating gas detection.

Conclusion

Although scientific research regarding gas sensing by layered nanostructure yielded appreciable progress over the last decade or so, resulting in newer, compact and efficient gas sensors, cost of such materials is still not attractive for large scale industrial production at many places. This is so because there are still many

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drawbacks such as wider bandgap, thermodynamic stability over narrower temperature range etc. limiting their space for better application. Lowering of detection limit, selective detection, and reduction in recovery time are still challenging and these require thoughtful engineering of the nanometric material through either increase in active site, tailoring the ease of charge transfer, usage of filters or change in ambience's wavelength by use of different monochromatic light etc. These trials need involvement of huge capital for successful development of appropriate gas sensors with better attributes. Ab-initio calculation offer a smarter choice for gathering useful information regarding feasibility and efficacy of any nanometric sensing material for detecting a particular gas or biomolecule by carrying out computer simulation which is much cheaper than practical experiment. Moreover, it is possible to interpret the sensing knowhow by postprocessing the simulation data which is helpful in deciding whether it is of worth to develop such gas sensor for practical purpose. The greatest advantage of such simulation method is that it can be done without any prior physical knowledge. In particular DFT is most popular for its accuracy and versatility over the others since it considers electron density as the variable and that is logical and consistent as per today's thought. Hence, theoretical simulation can be considered to be an indispensable part for sustainable development of novel layered nanostructured gas sensors.

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Conflict of Interest

It is hereby declared that there exists neither any known economic interest nor any conflict of interest.

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