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Modelling Simulation of Organic and Inorganic Interaction Based on First Principle Calculation

Tijjani Adam[1], Aeshah M. Mohammed[2], Mohammed Mohammed[3,] Omar S. Dahham[1], U. Hashim[3], Nik Z. Noriman[1]

[1]Faculty of Engineering Technology, Kampus Uniciti Alam Sg. Chuchuh, 02100 Padang Besar, Universiti Malaysia Perlis (UniMAP)
[2]University of Bagdad College of education for pure science Ibn-Alhaitham
[3]Center of Excellence Geopolymer and Green Technology, School of Materials Engineering, Universiti Malaysia Perlis, 01007, P.O. Box 77, D/A Pejabat Pos Besar, Kangar, Perlis, Malaysia
[4]Institute of Nano Electronic Engineering (INEE), 2Department of Electronic Engineering 01000 Kangar, Perlis, Malaysia

Abstract. The student presented theoretically interaction of organic and inorganic based on the electrostatic interaction created by the ssDNA interaction with sensor active surface, the ssDNA strand was immobilised on silicon-based sensor to create binding chemistry with subsequent target molecule. The sensor is influenced by the ability of the attached probe ssDNA to recognise it complements through matched and mismatched. Upon interaction, the electrical response of the sensor was calculated based on density functional. A growth exponential functional model was established with 5nA rate of growth indicating complementary reactive and the model equally generated revised degenerative mode with mismatched produce decaying exponential model, thus, with excellent prediction capability. The organic and in-organic material interactive model developed could be employed to test the experimental model to validate and predict the selectivity and sensitive of Nano based biosensors**.**

1. Introduction

Today, Nanowire devices have attracted wider attention among research communities, this argely due to its unique prospect properties in future application [1]. It has good electrical, optical magnetic properties, silicon nanowires in particular are largely employed in many applications. The electrons interaction size is important applications in smart sensors, storages and energy conversions. Thus, it is essential to understand using first principle without depending on experimental data to establish [2]. The electronics properties may differ when measured along different directions or planes within a crystal and strength electron interaction. Electrons have wavelike and particulate properties[3]. This indicated that electrons exist in orbitals defined by a probability. The total possibility of finding an interactive electron is depend on curvature of the nucleus (r) and this can be done through Schrödinger models[4]. Schrödinger equation the behavior of quantum system can be calculated and provide predictable results. Each orbital is located at a discrete energy level determined by quantum numbers and electron interaction is solely depending on distance. The model based on first principle means no equivalently or no adjustable parameters [5]. Therefore, the task is to understand and predict material properties without depending on exp. The atomic interaction becoming complicated as the number of

electrons increases because atomic interaction beyond the hydrogen atom is indeed complex but quite possible [5].

$$\hat{H} = T_e + T_N + V_{ee} + V_{eN} + V_{NN}$$

The complexity indeed rendered Schrödinger models not effective However, as stated the complexity can be solve by Born-Oppenheimer approximation. The Born-Oppenheimer approximation leads to a very important simplification of the wave function [6].

$$\hat{H} = T_e + T_N + V_{ee} + V_{eN} + V_{NN}$$

$$V_{ee} = \frac{1}{2}\sum_{ij(i\neq j)} \frac{e^2}{|r_i - r_j|} \quad V_{eN} = -\sum_{iI} \frac{Z_I e^2}{|R_I - r_j|} \quad V_{NN} = \frac{1}{2}\sum_{JI(I\neq J)} \frac{Z_I Z_J e^2}{|R_I - R_j|}$$

Thus, in this above assumption, the electron would be able to follow any movement of the nuclei quasi instantaneously and might then be basically moving in a constant field generated by the nuclei in eq. Although the Born-Opp. simplifies the original Shrö. eq. the electronic part in eq. above still only numerically solvable by introducing farther approximations. one fundamental approach to solve the electronic Shrö. eq. is the Hartree-Fock approach. The Hartree-Fock idea, its seeks to approximately finding solution to the electronic interaction, however, solving by it self without Schrödinger equation cannot clearly solve the equation and Schrödinger equation assumed that the wave function can be approximated by a single Slater determinant made up of one spin orbital per electron [1.2]. This will ensure the anti-symmetry of the wave function In H-F approach the exchange between electron as well as the correlated motion of electron of like spins due to the Pauli principle is taken into account [1-7]. Although H-F theory therefore contains a part of the correlation, the so-called Pauli correlation it is commonly agreed that the term correlation is used for all that is missing in H-F. An Alternative approach is given by density functional theory DFT. In DFT the central quantity is not the wave function, but the electron density n(r). So the this requirement call for understanding the Thomas-Fermi model. The Thomas-Fermi used n(r) of a system to calculate total energy used n(r) n(r) means the probability of finding any of the N electrons in a volume element dr_1. The N means the no of the electron [1, 2, 3-8].

$$T_{TF}[n] = C_F \int n^{5/3}(r) dr \qquad T = C_F \int \left[n(\vec{r})\right]^{5/3} d^3 r \qquad E_{TF}\left(n(r)\right) = K \int dr\, n^{5/3}(r)$$

Kinetic energy is a functional of the density and n(r) exhibits cusps only at the positions RA and the properties of each cusp related to the nuclear charge n(r) is sufficient to determine all properties of the system. The idea of Thomas-Fermi formulation for interactive total energy given isolated system in terms of its n(r) employing identical electron interactive model for K.E and treating the nuclear-electron attraction and e-e repulsion classically E_{TF}(n(r)= 3/10. However, the actual results obtained by their models for atoms are not accurate since there is neither exchange nor correlation included and the Thomas-Fermi K,E functional is only a very coarse approx. to the true K.E[8]. However, this approach does not predict molecular binding is predicted, which caused Thomas-Fermi model to be considered as of only little importance for giving quantitative results. Fortunately, the assumption was proven by Hohenberg-Kohn.

$$E[n(r)] = \int n(r) v_{ext}(r) dr + F[n(r)]$$

Hohenberg-Kohn state that every observable of a stationary quantum mechanical system can be calculated, in principle exactly, from the electronic ground-state density alone using the variational method involving only the density. The theorems indicate that within the BO approximation, the nuclear positions determinate the ground state of the system of the electrons Equally, the kinetic

energy of electrons can be calculated exactly from the wave function, rather than from the density. This was possible because of marrying wave function and density approach by Kohn and Sham

$$E[\rho] = T_e[\rho] + U_{ext}[\rho] + U_{ee}[\rho]$$

Where U_{ee} is the all electron-electron interaction potential E [ρ] is the Coulomb repulsion potential between the electrons. Following this approach the many body problem is again mapped into an effective single particle problem and all unknown terms into the exact correlation[9-13]. The one - particle wave function can now be determined by effective one particle equations under constraint to reproduce the density of the real , interacting systems. this yields the so-called Kohn-Sham equations. since the effective potential already depends on the density itself ,the Khon-Sham eq. have to be solved consistently within the K-S, LDA is based on Homogenous electron gas, which describes system of electrons in an infinity region of space with a uniform positive background charge to preserve overall charge neutrality Within the K-S formalism the K.E of the non-interacting system is only described using N one-particle wave functions [9-12].

$$v^{LDA}{}_{xc}(r) = \frac{\delta E^{LDA}}{\delta \rho(r)} = \varepsilon_{xc}(\rho(r)) + \rho(r)\frac{\partial \varepsilon_{xc}(\rho(r))}{\partial \rho(r)}$$

A notable improvement over the LDA is the generalized gradient approximation (GGA) obtained by expanding $E_{xc}[\rho]$ to the first order to consider both the density and its gradient.

$$E_{xc}^{GGA}[\rho, \mu\nabla\rho] = \int f(\rho, \nabla\rho)dr$$

2. Results and Discussion

A change in the conductance of silicon nanowire because the induced partial charge was computed through the simulations. A comprehensive simulation framework was developed involving the simulation of silicon nanowire using the finite element method and calculation of the partial charge due to DNA hybridization using molecular dynamics simulator. The effects of hybridization induced partial charge on the interaction between organic molecule (DNA) and inorganic biosensor was investigated through the simulation of nanowire using COMSOL Multiphysics and the simulation of DNA using molecular dynamic simulation (MD) (Al-mufti et al., 2013). These two simulations are integrated to develop an overall simulation framework. These simulations were done in three steps. In the first step, only biosensor was used without any DNA molecules. In the second step, the simulation of biosensor with probe ssDNA was performed. Due to the partial charge of ssDNA, the conductance of silicon nanowire was affected. Finally, the third step involved hybridization between probe ssDNA and the target ssDNA molecules. In these steps, the partial charge induced due to hybridization of complementary ssDNAs caused a significant change in the conductance of silicon nanowire. In these simulations, COMSOL Multiphysics were used for the simulation of inorganic part called nanowire biosensor. The partial charge due to ssDNA and dsDNA molecule was computed using molecular dynamics (MD) simulation.

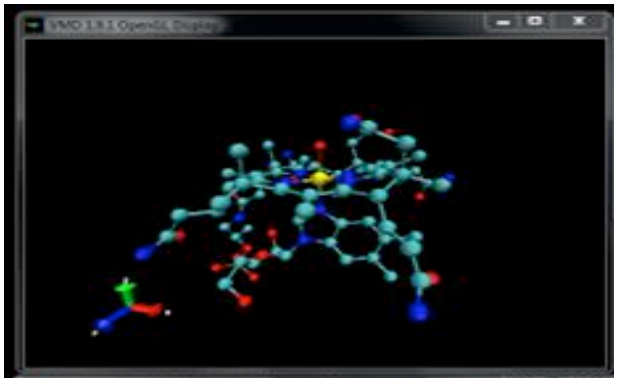

Figure 1 : interaction between organic and in organic

The system of bio-sensor is influenced by ligand pair, In the figure 1. A functional bio-interface layer surrounding the oxide layer has receptor bio-molecules probe and a thickness of 5 nm. The last layer is referred to as an electrolyte of 80 nm width in which the whole system was immersed. The corresponding dielectric constant characterizes each layer as a continuum medium. Electric property is a basic dependent variable in the system. The potential is distributed throughout the system of bio-sensor. The calculation of the finite element was used for its estimation in which a boundary condition results from the bio-interface surface charge. With the availability of potential distribution, there is an estimation of other quantities including a conductance, as presented in the following sections.
The PDE regenerated was used for the simulation of the model. The electrostatic model is a simplified form of the nanowire silicon model. The electrostatic equations are a complex system of nonlinear, partial-differential equations (PDE).

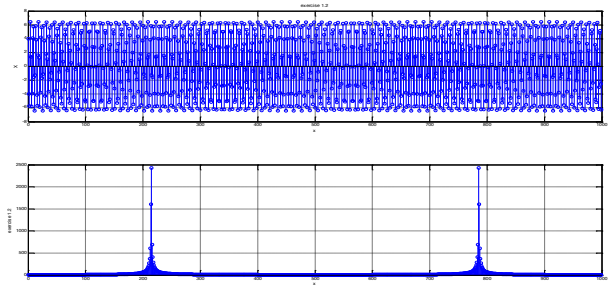

Figure 2 : Atomic Interaction

As mentioned, the biosensor interaction occurred as result of four regions namely, silicon nanowire, oxide layer, functional layer bio-interface and the analyte. The study explored the impacts on layers in order to gain better understanding of the interaction between nanowire and DNA. Fig.2 The detailed simulations of silicon nanowire and oxide layer are required to get a high conductivity and sensitivity that can get a sensor and then get an interaction with organics. The third layer is a linker and bio-interface molecule as an important layer to make an interaction between nanowire and DNA target. An electrolyte is a substance that ionizes when dissolved in suitable ionizing solvents such as water with the most soluble salts, acids, bases, and gases, such as hydrogen chloride, dissolution of some biological DNA. In those layers, physical and chemical properties are governed by a number of constants and variables. Among them, $\phi(\vec{r})$ is the electrostatic potential, and n_0, p_0 and c_0 represent, respectively, the initial electron concentration, initial hole concentration and equilibrium charge concentration. Also, k_B is the Boltzmann constant; and T represents the absolute temperature. Permittivity of silicon nanowire, functional layer and the electrolyte are given by $\varepsilon_{Si}, \varepsilon_{Fn}$, and ε_{El}, respectively.

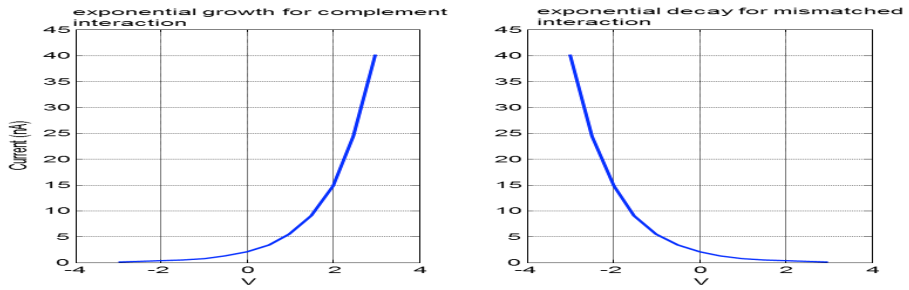

Figure 3 : Show the mismatched and complement with decay and growth current curve

The potential distribution in the extracellular medium described by the electrostatic form of the equations is solved using the electrostatic and the second PDE, a general form. The nonlinear differential equations describing the membrane behavior are coupled with the FEM solution, called Boundary Conditions. Also, coupling is achieved by setting the boundary conditions (BC), as given below. All boundaries of the cuboids axon in the PDE subdomain are viewed as Neumann BCs; the normal component of the electric potential is zero

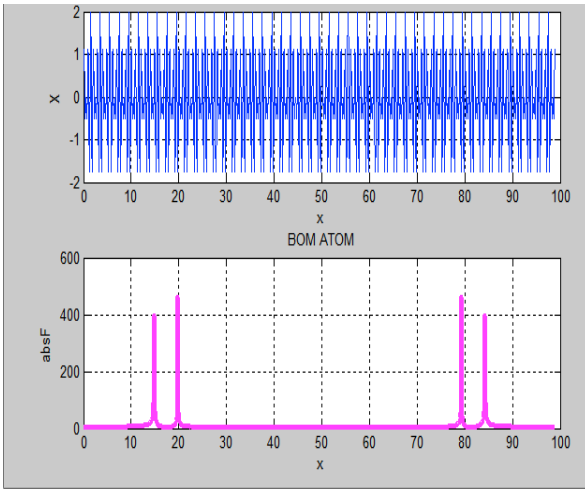

Figure 4 : Complément and mismatched atomic interaction

The mismatched and complement for ssDNA hybridization using molecular interactive model is establisshed. In that hybridization process, two complementary ssDNA interacted to form redable dsDNA. The partial charge was generated in this hybridization process as shown in fig.4. For convenience, a suitable force field was used and calculated in the design and simulation of single strand NDA using molecular dynamics method. In each of these steps, the partial charge was computed for corresponding DNA using a suitable force field. Nevertheless, MD simulations can delineate the atomistic details of the DNA system because they compute atomic trajectories by solving the equations of motion using empirical force fields that describe the actual atomic force in bimolecular systems.

3. Conclusion

The study demonstrated the theoretically interaction model of organic and inorganic based on the electrostatic interaction created by the ssDNA interaction with sensor active surface, the ssDNA strand was immobilised on silicon based sensor to create binding chemistry with subsequent target molecule. The sensor is influenced by the ability of the attached probe ssDNA to recognise it complements through matched and mismatched. Upon interaction, the electrical response of the sensor was calculated based on density functional. A growth exponential functional model was established with 5nA rate of growth indicating complementary reactive and the model equally generated revised degenerative mode with mismatched produce decaying exponential model, thus, with excellent

prediction capability. The organic and in-organic material interactive model developed could be employed to test the experimental model to validate and predict the selectivity and sensitive of Nano based biosensors. a model based electrostatic principle which is responsible for signal generation upon DNA interaction

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