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NANOTRANSISTOR MODELING WITH MoS_2 CHANNEL

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Modeling of semiconductor carrier transport properties based on the drift-diffusion model is one of emerging activity of computational electronics. The p-n junction between materials with different type of conductivity can set up an internal electric field, which is responsible for separation of charge pairs electron and hole. The distribution of electric field in the depletion layer can be obtained by solution of Poisson's equation. Although this equation does not appear to have an analytical solution, numerical treatment offers a deeper comprehension of the structure, achieving a complete control on the various parameters and defining their role in the device operation. The molybdenum dichalcogenides belong to the large family of layered transition metal dichalcogenides whose crystal structure from the stacking of sheets of hexagonally packed atoms.
Keywords: modeling, structure, transport properties, lattice

I. Molecular structure

The bulk MoS_2 has a hexagonal and the space group of unit cell is P63mmc(196). The experimental lattice parameter and the a/c are 3.160Á and 12.294Á. The crystal structure of MoS_2 consist of a Mo atom layer sandwiched between two S layers in a trigonal-prismatic arrangement.

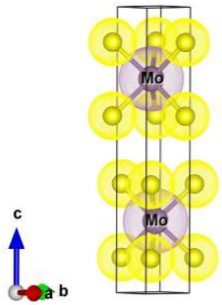

Figure 1. 3D structure of trigonal-prism coordinated unit cell.

II. Calculation Method

First-principles total energy calculations using the Plane Wave self-consistent field (PWscf) method. Wave function plane waves up to a kinetic energy cutoff of 30 Ry Charge density plane waves up to a kinetic energy cutoff of 450 Ry Perdew Wang -91 (PW91) type of exchange correlation functional Ultrasoft pseudopotentails for ionic potentials 4 x 4 x1 supercell, 2 x 2 x1 Monkhort — Pack mesh for k-point in bulk and monolayer(ML) respectively Electronic occupation -Gaussian distribution with an electronic temperature of KT=0.001 Ry Optimazition until forces are less than 0.05 eV/A

III. Pure MoS_2

The MoS_2 unit cell to multiple 4:4:1 scale has created a tier 48 atomic structure. Chemical structure simple molecular lattice is simulated by a program called a Vesta.

IV. N and p type MoS_2

Wechoosebinaryinorganiccompound Molybdenym disulfide[MoS_2], with the substitutional nitrogen[N], and flourine[F] doping.

V. p-n type MoS_2

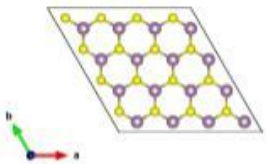

Figure 2. 48 atom with mono layered MoS_2 structure.

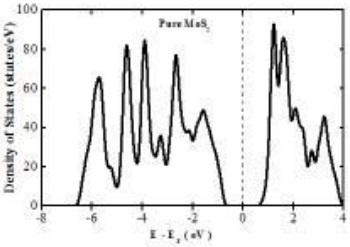

Figure 3. Pure MoS_2 of density of states. The vertical dashed line is Fermi level.

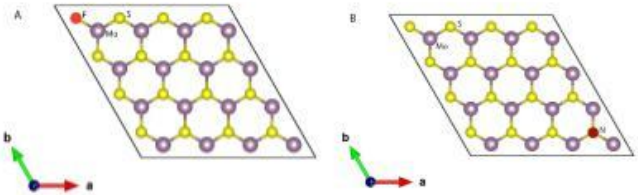

Figure 4. The 2D F & N doped MoS_2 structure. Figure 4[a]. F doped MoS_2 and Figure 4[B]. N doped MoS_2

We implemented the GPU-based calculation diode IV characteristic of p-n junction based the MoS_2. To calculate density of state we used Quantum espresso run on the CPU.

	Band gap (eV)
Pure MoS_2	1.769 eV
F doped MoS_2	1.7 eV
N doped MoS_2	1.65 eV
F & N doped MoS_2	1.42 eV

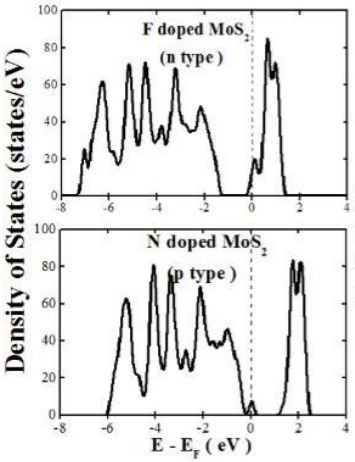

Figure 5. Density of states of F doped MoS_2 and N doped MoS_2

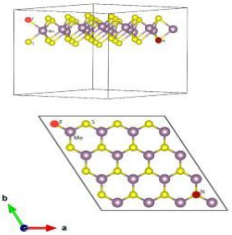

Figure 6. The positions of H and V vacancy in F & N doped MoS_2

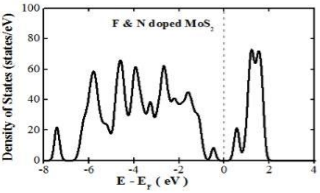

Figure 7. Density of states of F & N doped MoS_2

VI. MoS2 p-n junction I(V) characteristic

If we give V potential in p-n junction electrochemical potential difference will be μ1-$\mu_1 - \mu_2$ = qV. Density of state will be increased from the external voltage influence (Figure 3. Graph of density of state) therefor change will be occurring in the density of electron charge.

$$J_p(x_{n0}) = \frac{Q_p}{A\tau_p} = e\frac{D_p}{L_p}p_{n0}(e^{eV_a/(k_BT)} - 1)$$

We took three parameters: diffusion length Lp, external voltage Va to change the value in determining range to end the I(V) characteristic of p-n junction. This work allows calculating the current simulation in the accuracy of nanometer scale.

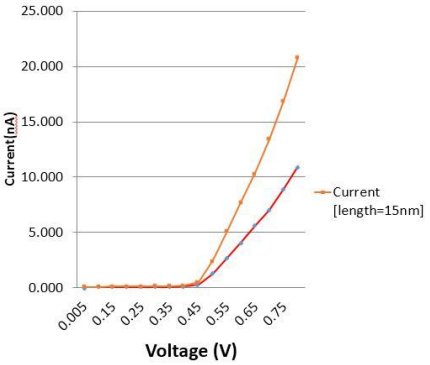

Figure 8. I(V) characteristic of p-n junction

Summary

N doped MoS_2 and F doped MoS_2 of graph of density of states energy level relation. N and F doped MoS_2p — n junction semiconductor diode. From the view of graph it is V b^{uilt} is 0.4V and it is same us a general curve od diode characteristic.

Acknowledgments

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МОДЕЛИРОВАНИЕ НАНОТРАНЗИСТОРА С ПОМОЩЬЮ MoS_2 КАНАЛА

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Моделирование транспортных свойств полупроводникового носителя на основе модели дрейфа-диффузии является одним из передовых в вычислительной электронике. P-n переход между материалами с различным типом проводимости может создать внутреннее электрическое поле, которое отвечает за разделение пар зарядов электрона и дырки. Распределение электрического поля в обедненном слое может быть получено путем решения уравнения Пуассона. Хотя это уравнение не имеет аналитического решения, численное решение предлагает более глубокое понимание структуры, достигает полного контроля над различными параметрами и определяет роль этих параметров в процессе работы устройства. Молибденовые дихалькогениды принадлежат к большому семейству слоистых переходных металлов дихалькогенидов, кристаллическая структура которых имеет шестиугольную упаковку атомов.

Ключевые слова: моделирование, структура, транспортные свойства, решетки