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OPTICAL PROPERTIES OF LOW-DIMENSIONAL SYSTEMS: METHODS OF THEORETICAL STUDY OF 2D MATERIALS

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Heterostructures based on graphene and two-dimensional films of nanostructured, ferromagnetic, transition metal oxides are promising for the development of new multifunctional materials for memory cells, quantum computer elements, Li-battery anodes, (photo) catalysts, supercapacitors, transistors, sensor materials, solar panels, fuel cells, electrochromic devices. A large volume of publications devoted to graphene and heterostructures based on it is and mainly their synthesis processes of hybrid structures. The methods of theoretical investigation of the optical properties of two-dimensional film materials, despite their diversity, require improvement. Consequently, the article presents methods of theoretical investigation of the optical properties of two-dimensional hybrid film structures in combination with ab-initio method.

Keywords: *heterostructures, two-dimensional materials, low-dimensional structure, transition metal oxides, Van der Waals materials.*

INTRODUCTION

The discovery of semi-metallic graphene, which is a two-dimensional allotropic modification of carbon formed by a carbon layer one atom thick, created a powerful theoretical and experimental prerequisite for the development of two-dimensional film materials (2DLM). Each film contains a cell with a covalent bond providing a stable configuration of the structure. Hexagonal BN (boron nitride) called white graphene is a close analogue of graphene with a similar geometric structure, in a primitive cell of which each carbon atom is replaced by boron and nitrogen. Hexagonal BN being a wide-band insulator is used as thin tunnel barriers [1, 2], sealing materials [3] and nondefective dielectrics [4]. Currently, experimental work is being developed on synthesizing films with controlled electronic properties with a combination of carbon, nitrogen and boron.

Another group 2DLM – transition metal dichalcogenides (TMD) contains a variety of film materials with tunable electronic properties and different band gap widths. It is generally denoted AB_2, where A metal is mainly molybdenum or tungsten, and B is chalcogenide (sulfur, selenium or tellurium), which are exfoliated from natural ores or synthesized by chemical vapor deposition. Along with molybdenum and tungsten, stable compounds with zirconium, ruthenium, tantalum, titanium, niobium and nickel are used. Of the many compositions, the well-studied compositions MoS_2, $MoSe_2$, WS_2 and WSe_2 have a configurable band gap of ~1–2 eV with carrier mobility of 100 $cm^2 \cdot V^{-1} \cdot s^{-1}$ at room temperature [5].

Black phosphors or phosphorene (in the form of a monofilm) have high anisotropic properties and a tunable band gap from 0.33 eV to 1.5 eV with carrier mobility of 1.00 $cm^2 \cdot V^{-1} \cdot s^{-1}$ at room temperature [6].

Two-dimensional transition metal oxide films (TMO) are currently important both in fundamental research and in technological applications due to their wide range of material properties from semiconductors, metals to superconductors. However, a material with fixed properties may not have universal application. Due to the unique crystal structures, physical and chemical properties, 2D TMO can be efficiently configured using various strategies such as size reduction, intercalation, heterostructure, doping and gating. The structures created by the combination of two or more atomically thin graphene-like materials change the properties of the initial structures, and a material with new hybrid properties appears, which opens up new paradigms for the development of new materials and nanodevices. Strong covalent bonds ensure the planar stability of 2D crystals, and the connection between different layers is provided by van der Waals interactions. Hence, such heterostructures are called van der Waals vdW heterostructures.

Heterostructures based on graphene and two-dimensional films of nanostructured transition metal oxides are promising for the development of new multifunctional materials for memory cells, quantum computers, anodes of Li-batteries, (photo)catalysts, supercapacitors, transistors, sensor materials, solar panels, fuel cells, electrochromic devices. A large volume of publications devoted to graphene and heterostructures based on it is practically devoted to the study of the features of the synthesis processes of hybrid structures. The combination of graphene and two-dimensional nanostructured transition metal oxides will lead to fundamentally new and unidentified processes, patterns at the interface of structural elements, creating a new base for multifunctional materials in the nanoscale range.

The creation of two-dimensional (2D) materials has been promising since the invention of graphene. Two-dimensional transition metal oxides films (TMO) are currently important both in fundamental research and in technological applications due to their wide range of material properties from semiconductors, metals to superconductors. However, a material with fixed properties may not have universal application. Due to the unique crystal structures, physical and chemical properties, 2D TMO can be efficiently configured using various strategies such as size reduction, intercalation, heterostructure, doping and gating. Due to the flexible adjustment of the properties of 2D TMO, they become attractive candidates for various applications, including electronics, optoelectronics, catalysis and energy.

However, all these 2D films are simple semiconductors or semi-metals in which charge is the dominant degree of freedom. Other functional properties, such as magnetism and polarity, due to other degrees of freedom (for example, spin, orbit and lattice), are usually inactive or insignificant in these systems, which limits the scope of their application. Although many ab initio calculations and some precise experiments have claimed that magnetism in 2D materials is induced by surface relief, boundary conditions, doping, defects, or a displaced electric field, these types of magnetism are somewhat external. Despite enormous efforts, these types of external magnetism caused by external factors are still hindered by their weak magnetization, low operating temperature, poor reliability and uncontrollability. We review the recent progress and challenges, and offer our perspective on the exploration of 2DLM-based vdWHs for future application on oxygen evolution reaction (electrode/catalyst functionalities) and optoelectronics.

Brief review of theory of experimental methods of studying vdW

Two-dimensional Van der Waals (vdW) graphene-TMO materials have multielectronic effects in 2D layers that create unstable collective states. Due to this, ferromagnetic ordering of spins was observed in 2D soft ferromagnets at low Curie temperatures. The inclusion of stable collective states will expand the technological application of this class of materials.

Experimentally [7, 8] it was revealed that in transition metal oxides (TMO) in combination with graphene at the interface of the structure forms new and promising magnetic, electronic and optical properties. In low-dimensional structures, the localization region of wave functions is tens of nanometers, the matrix elements of the interband transitions have the same dimension as the width of the structure. This in turn enhances the optical response in such structures as opposed to 3D structures. Since 2 materials of the system are one atom, their surface conductivity tensor is described in *xy* planes as

$$\gamma = \begin{bmatrix} \gamma_{xx} & \gamma_{xy} \\ \gamma_{yx} & \gamma_{yy} \end{bmatrix}$$

Here the *z*-axis components disappear, which $\gamma_{zz} = \gamma_{xz} = \gamma_{yz} = 0$. Considering magneto-optical effects [9–11], the surface conductivity tensor is represented as

$$\gamma = \begin{bmatrix} \gamma_L & \gamma_H \\ -\gamma_H & \gamma_L \end{bmatrix} \quad (1)$$

where γ_L longitudinal conductivity and γ_H The Hall conductivity was defined by the Kubo formalism [12]. At room temperature and in the mid-infrared region, the longitudinal conductivity and γ_H Hall conductivity is related with the Drude model [13] by the following expressions:

$$\gamma_L = \bar{\gamma}\frac{1 - iw\tau}{(w_c\tau)^2 + (1 - iw\tau)^2}, \quad (2)$$

$$\gamma_H = \bar{\gamma}\frac{w_c\tau}{(w_c\tau)^2 + (1 - iw\tau)^2}, \quad (3)$$

where $\tau = \frac{1}{2\Gamma}$ – scattering time (Γ – the rate of attenuation of plasmons), $\omega_c \approx eB_z v_F^2 / \mu_c$ cyclotron frequency (electron charge *e*, B_z component on the axis *z* of magnetic field), $v_F \approx 10^6 m/s$ Fermi speed,

$$\bar{\gamma} = \frac{2e^2\tau k_B T}{\pi\hbar_2}\ln\left[2\cosh\left(\frac{\mu_c}{2k_B T}\right)\right]. \quad (4)$$

For frequencies above the mid-infrared region, the main expression of [8] longitudinal and Hall conductivity are not simplified in the Drude model. In the case of magnetostatic simplification $(B_z = 0)$, longitudinal conductivity $\gamma_L = \gamma_{intra} = \gamma_{inter}$ because of the intra-cavitary (γ_{intra}) and interpolar γ_{inter} contribution

$$\gamma_{intra}(w) = \frac{2e^2 k_B T}{\pi\hbar}\frac{\tau}{1 - iw\tau}\ln\left[2\cosh\left(\frac{\mu_c}{2k_B T}\right)\right]. \quad (5)$$

Interband conductivity is formed from direct interband electronic transitions. It is not taken into account at room temperature and frequencies below the mid-infrared zone, since it is much smaller than the interband contributions. It is expressed in integral form:

$$\gamma_{inter}(w) = \frac{e^2}{4\hbar}\left[G\left(\frac{w}{2} + \frac{4iw}{\pi}\int_0^\infty \frac{G(s) - G(w/2)}{w^2 - 4s^2}ds\right)\right], \quad (6)$$

$$G(s) = \frac{\sinh[\hbar s/(k_B T)]}{\cosh[\mu_c/(k_B T)] + \cosh[\hbar s/(k_B T)]} \quad (7)$$

in optical properties are described they are treated as surfaces. When exposed to an electric field, a nonlinear optical response is manifested. For the first time, the

nonlinear optical response in solids and liquids was investigated by J. Carom.

In many computational electromagnetic methods, it is more convenient to work with volumetric equivalents of surface quantities. In practice, volumetric conductivity is used instead of surface conductivity $\gamma_b = \gamma_L / h_{eff}$, where h_{eff} the effective thickness is 2DLM. The electromagnetic properties of such materials are also described by the dielectric permittivity ε which is related to conductivity with the following expression:

$$\varepsilon_r = 1 + \frac{i\gamma_h}{\varepsilon_0 w} = 1 + \frac{i\gamma_L}{\varepsilon_0 w h_{eff}} \quad (8)$$

$$\varepsilon_r = 1 + \sum_{k=1}^{N} \frac{f_k}{w_k^2 + iw\delta_k + (iw)^2}, \quad (9)$$

where f_k, w_k and δ_k oscillation strength, resonant frequency and spectral width.

Along with linear optical properties, nonlinear optical properties of low-dimensional structures by the nonlinear surface conductivity tensor $\gamma_x^{(n)}(\Omega, w)$, where $\Omega = nw$ and $n = 2,3,\ldots$. The surface conductivity tensor of the third harmonic of graphene is expressed as:

$$\gamma_x^{(3)}(3w, w) = \frac{i\gamma_0 (\hbar v_F e)^2}{48\pi(\hbar w)^2} T\left(\frac{\hbar w}{2|\mu_c|}\right), \quad (10)$$

Van der Waals (vdW) heterostructures consist of two-dimensional (2D) materials and functional different structures (transition metal oxides, organic molecules, layered metal oxides, layered double hydroxides, layered metal chalcogenides, layered metal carbides and etc) which have been intensively studied for development optoelectrical properties [9]. If the functional structures are appropriately designed, this enables manipulation of the electronic structure and optical properties of 2D materials [10]. To determine the effectiveness of mixed-dimensional heterostructures, it is important to understand the nature of charge and energy transfer processes across the semiconductor interface at fundamental timescales. It was discussed the recent findings on photophysical processes within three different vdW heterostructures: 1) conjugated polymer/MoS2 organic/2D heterostructures [11]; 2) polymer: fullerene/MoS2 organic/2D heterostructures in the presence of a plasmonic metasurface [12]; and 3) ReS2/MoSe2 type-II 2D/2D heterostructures [13–16]. In the organic/2D heterostructures investigated, ultrafast charge transfer from MoS2 to the conjugated polymers occurred within 9 ps, and in some cases, in under 120 fs. The charge generation yield was improved by over a factor of 6 at ultrafast time scales in the presence of a plasmonic metasurface. In the ReS2/MoSe2 heterostructure, we show that resonant energy transfer dominates over charge transfer from ReS2 to MoSe2, even without a charge-blocking interlayer. vdW heterostructure Hybrid Materials with different energy application purposes with anisotropic 2D nanosheets of layered inorganic solids (layered metal oxides, layered double hydroxides, layered metal chalcogenides, layered metal carbides, and graphene) attract research interest therefore of their multifunctional nanohybrids applicable for renewable energy technologies [17–20]. The monolayered 2D nanosheets of inorganic solids can be synthesized by soft-chemical exfoliation reaction of the pristine layered materials. A great diversity in the chemical compositions, crystal structures, and defect structures of inorganic nanosheets provides this class of materials with a wide spectrum of physical properties and functionalities. The inorganic nanosheets can be used as powerful building blocks for exploring high performance hybrid electrodes and catalysts with the help of interface and defect engineering. These materials can play a role as active components, additives, and substrates for improving the energy performance of hybridized species. In this talk, several practical examples of interface-/defect-engineered 2D inorganic nanosheet-based hybrid materials with electrode/catalyst functionalities will be presented together with the discussion about the relationship between chemical bonding nature and functionalities. Perovskite structures are promising materials for energy purpose systems and with combination with graphene used for as solar collectors, with their complexity structure and electronic and optoelectronic properties its required investigation as electrode/catalyst materials.

Computational methods for 2DLMs

Calculations will be performed within the framework of density functional theory (DFT) [21], DFT+U, [22, 23] in the software that perform quantum-chemical calculations. One of them VASP software package. The study uses an integrated approach that includes the search and preparation of nanoclusters of the systems under consideration, descriptions and characterization of the structure and size by additional computational methods, calculation of electronic properties, visualization of the results obtained, as well as comparison of computational and experimental data. However, the accuracy of DFT depends on the correct choice of the exchange-correlation functional [24–27]. The theoretical study of the relaxation of the geometry of the structure and electronic excitation is a developing task. Computational ab initio methods have proven to be a reliable tool in the study of spectral dynamics. The brief explanation of the computational method of identifying optical properties of 2D structures given in Figure.

As seen from the scheme relaxed structures taken from the computational 2D materials database (C2DB) [24] and on next step calculated electronic band energies and wave functions with DFT calculations. Also performed calculations to obtain the optical vibrational modes. The momentum and electron-phonon matrix elements that taken from electronic states and phonon modes analyzed and stored. At the end of calculations for a considered excitation frequency and input/output

polarization vectors the Raman spectrum is calculated. Experimentally Raman spectroscopy is mainly used to reveal composition, structure and layer thickness of 2D materials. Authors [29] performed computational identifying 733 2D materials from C2DB for Raman spectrum and compare them with experimental data for 15 known monolayers [30]. By them illustrated dates in article for MoS_2 (H-phase) and WTe_2 (T'-phase). Calculated spectra dates show precious agreement with experiments for the Raman peak positions [31].

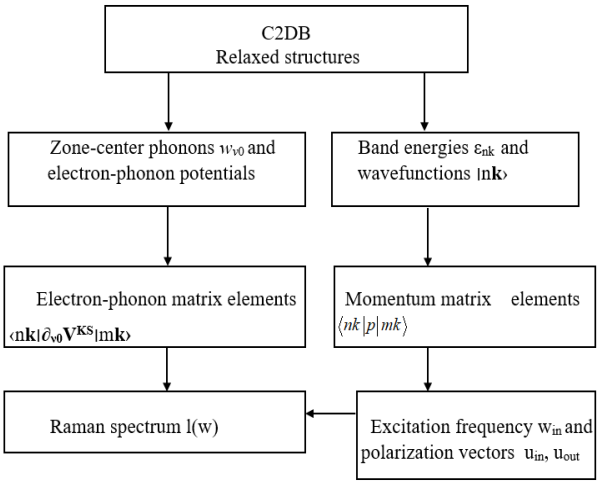

Figure. Computational method scheme of the calculation Raman tensor of 2D materials

At the moment, this method is in the early stages of development. Thus, now there are no commercial and public programs on which it would be possible to calculate the spectral dynamics. Preliminary steps have been implemented in programs in the form of conventional additions that import information about molecular dynamics and the electronic structure for these configurations from standard quantum software packages of quantum chemistry and then build spectral dynamics based on these inputs. In modern modeling methods, photoexcitation or injection of charge carriers puts the system into a nonequilibrium state causing spectral dynamics, which is described by solving the corresponding nonstationary Schrodinger equation or the Liouville-Neumann equation for a reduced density matrix with certain approximations. This atomistic method involves interactions of electronic degrees of freedom with lattice vibrations. The implemented method describes dissipative quantum dynamics of electrons by combining a density matrix for open systems of electronic excitations at the semiconductor-metal interface. This combination of methods has the potential to describe a wider range of phenomena with higher accuracy [32–33].

Studying the energy of oxide materials, one can imagine photoinduced catalysis as a sequence of elementary atomistic interactions between electrons, lattice vibrations, and external illumination. In these reactions, the electronic system is not isolated. The initial goal is to study the interaction of electronic excitation with lattice vibrations. The atomistic electronic structure approach is important for studying bounded systems with reduced symmetry (inhomogeneous systems, surfaces with defects, nanoparticles), since standard approaches are unable to investigate periodic structures. The available atomistic treatments of the interactions of electrons with ionic skeletons suggest a "continuous" calculation of the non-adiabatic interaction. We found a slight difference between the estimates of the interaction energy obtained by the two methods. Using this methodology, we expect to significantly reduce the required numerical and time resources and speed up the computational procedure.

The problem of the band gap width is caused by the local nature of the exchange energy (within LDA or GGA). The Hartree-Fock approximation ignores correlation, but includes exact exchange, whereas DFT approximates electronic exchange and correlation, which leads to the so-called exchange-correlation functional. Hybrid exchange-correlation functionals, such as those constructed by Purdue et al. [34], which combine the exchange correlation of GGA with the exact exchange of HF, seem to be suitable for semiconductors.

Perspectives

The development and research of nanoscale van der Waals heterostructures from (2D) films of transition metal oxides (OPM) and layered structures based on them as promising materials for micro-, nano- and optoelectronics is a rapidly developing direction in science. Theoretical at the atomic level, 2D films are being developed from epitaxial ultrathin oxide layers on various substrates with varying amounts of film to study their chemical properties and structure.

The theoretical predestination of the electron-optical and magnetic properties of the above materials will allow us to characterize the structures of defects in transition element oxides and develop methods for controlling them in the process of manufacturing electronic devices with the required properties.

Despite of the tremendous quantity of research activities of 2DLMs with variable electronic properties and the unique ability to exfoliate and restack 2DLMs hybride structures as vdW nowadays required detailed study for materials engineering and device design. By combining 2D semiconductors with low dimensional materials, mixed-dimensional heterostructures benefit from the advantageous properties of their constituent components. Recently researches devoted to TMO, organic molecules, layered metal oxides, layered double hydroxides, layered metal chalcogenides, layered metal carbides and etc. Perovskite structures with complexity of structure is perspective objects for studying for combination with graphene like low dimensional systems for creation the van der Waals hybrid heterostructures. Therefore, the task of development and research of hybrid van der Waals structures based on pervskite is still open. To determine the effectiveness of analogy mixed-dimensional heterostructures, it is important to under-

stand the nature of charge and energy transfer processes across the semiconductor interface at fundamental timescales. In further researches we aimed to study different perovskite structures with combination low dimensional systems like graphen.

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ТӨМЕН ӨЛШЕМДІ ЖҮЙЕЛЕРДІҢ ОПТИКАЛЫҚ ҚАСИЕТТЕРІ: 2D МАТЕРИАЛДАРДЫ ТЕОРИЯЛЫҚ ЗЕРТТЕУ ӘДІСТЕРІ

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Графен негізіндегі гетероқұрылымдар және наноқұрылымды өтпелі металдардың ферромагниттік оксидтерінің екі өлшемді пленкалары жад элементтері, кванттық компьютер элементтері, литий-ионды батарея анодтары, (фото) катализаторлар, суперконденсаторлар, транзисторлар, сенсорлық материалдар, күн панельдері, отын элементтері, электрохромдық құрылғылар үшін жаңа көп функциялы материалдарды әзірлеуге перспективалы болып табылады. Зерттеулердің үлкен көлемі графен мен оның негізіндегі гетероқұрылымдарға және негізінен оларды гибридті құрылымдардан синтездеу процесіне арналған. Екі өлшемді пленка материалдарының оптикалық қасиеттерін теориялық зерттеу әдістері, олардың әртүрлілігіне қарамастан, жетілдіруді қажет етеді. Осылайша, мақалада ab-initio әдісімен біріктірілген екі өлшемді гибридті пленка құрылымдарының оптикалық қасиеттерін теориялық зерттеу әдістері келтірілген.

Түйін сөздер: *гетероқұрылымдар, екі өлшемді материалдар, төмен өлшемді құрылым, өтпелі металл оксидтері, Ван дер Ваальс материалдары.*

ОПТИЧЕСКИЕ СВОЙСТВА НИЗКОРАЗМЕРНЫХ СИСТЕМ: МЕТОДЫ ТЕОРЕТИЧЕСКОГО ИССЛЕДОВАНИЯ 2D МАТЕРИАЛОВ

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Гетероструктуры на основе графена и двумерных пленок наноструктурированных ферромагнитных оксидов переходных металлов перспективны для разработки новых многофункциональных материалов для элементов памяти, элементов квантового компьютера, анодов литий-ионных батарей, (фото) катализаторов, суперконденсаторов, транзисторов, сенсорных материалов, солнечных панелей, топливных элементов, электрохромных устройств. Большой объем публикаций посвящен графену и гетероструктурам на его основе и, главным образом, процессам их синтеза из гибридных структур. Методы теоретического исследования оптических свойств двумерных пленочных материалов, несмотря на их разнообразие, требуют совершенствования. Следовательно, в статье представлены методы теоретического исследования оптических свойств двумерных гибридных пленочных структур в сочетании с методом ab-initio.

Ключевые слова: *гетероструктуры, двумерные материалы, низкоразмерная структура, оксиды переходных металлов, материалы Ван дер Ваальса.*