Research of hybrid perovskite - low dimensional materials

Balzhan Satanova[1], Fatima Abuova[1], Gulbanu Kaptagay[2], Nurgali Koilyk[2], Aisulu Abuova[1]
[1]L. N. Gumilev Eurasian National University, Astana, Kazakhstan
[2]Kazakh National Teacher Training University, Almaty, Kazakhstan

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). In other hand, 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 provided by van der Waals interactions. Hence, such heterostructures are called van der Waals vdW heterostructures [1].

Heterostructures based on graphene and two-dimensional films of nanostructured ($BaTiO_3$), ferromagnetic ($La_{2/3}Sr_{1/3}MnO_3$, $SrRuO_3$), 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. These 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. In presented paper the heterostructures on the base of from perovskite and layered structure was simulated and considered electronic, optical and properties for energetical applications with ab-initio methods.

It was predicted that the creation and management of such d-states could be realized by introducing impurities into the TMO. In our work, the necessary TMO with unique properties created in this way will be an object for substantiating various physical and chemical properties.
Also, during the project implementation, it is important to determine, in accordance with the Mermin-Wagner theorem [14], whether a stable state of symmetry is maintained at a finite temperature in systems with sufficiently short-acting interactions at dimension $d \leq 2$. Consequently, short-acting fluctuations are less preferable from an energy point of view.

The proposed goals and methodology will allow us to advance in understanding the existing problems in the study of quantum (film) materials. In particular, this will allow us to study the mutual influence of spontaneous ordering in the TMO with a decrease in the sample dimension.

First of all, it should be noted that all calculations will be performed within the framework of density functional theory DFT, DFT+U in the 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.

References

[1] A Soumyanarayanan andet al. Nature.-2016.-Vol. 539.-P.509

Satanova Balzhan was born on 19.05.1994 in the Merken District of Taraz Republic Kazakhstan. In 2001, went to school No. 17 named after Trubitsyn,in 2013 entered the Bachelor's degree in “Nuclear physics” of the Faculty of Physics and technology L N. Gumilyov Eurazian national university, Department of Nuclear Physics new materials and technologies. In 2018, received a master's degree in nanotechnology and nanomaterials. Since 2021 studyies for a doctoral degree in nanotechnology and nanomaterials.
Presentationg author: Balzhan Satanova
e-mail of presenting author: clever_s.balzhan@mail.ru tel:+7-707-982-02-77