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INVESTIGATION OF THE INFLUENCE OF SET PARAMETERS ON THE ACCURACY WITH MODELING THE BAND STRUCTURE OF KF AND LiF CRYSTALS

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Аннотация. Берілген жұмыста 0 К температура жағдайында түрлі кеңістіктік топтардағы KF және LiF нанокристалдарының зоналық құрылысының компьютерлік модельдеуінің нәтижелері көрсетілген. Есептеу уақытын үнемдеу мақсатында тек қана байланыстыруға қатысатын электронды санайтын, арнайы жалған потенциалдар қолданылды. Көрсетілген жұмыстағы барлық есептеулер жоғары спиндік ферромагниттік инициациясы бар магниттік иондарда спиндік поляризацияны қолдану жолымен жүргізілді. Берілген сипаттамалардың модельденуі Burai 1.3 бағдарламалық пакетінде, сонымен қатар CIF файлдарды генерациялауға мүмкіндік беретін materialsproject.org компьютерлік сайтында жүзеге асырылды. Зерттеу жұмыстарының барысында жалған потенциалдарды қолдану әсерінен электрондар мөлшерінің азайғаны, сонымен қоса жазық толқындар негізінде жүзеге асатын есептеулерде ерекше мәнге ие болған, қажетті бөлшектеу энергиясының да қысқарғаны анықталды. Алынған нәтижелер фундаменталды болып табылады және нанокристалдарды зерттеуде пайдалы болуы мүмкін.

Түйін сөздер: KF және LiF нанокристалдары, зоналық құрылыс, күй тығыздығы, толық энергия, компьютерлік модельдеу.

Аннотация. В работе представлены результаты компьютерного моделирования зонной структуры нанокристаллов KF и LiF в различных пространственных группах при температуре 0 К. Для сокращения вычислительного времени использовались псевдопотенциалы, которые учитывали только участвующие в связывании электроны. Все расчеты в данной работе были выполнены с использованием спиновой поляризации на магнитных ионах с высокой спиновой ферромагнитной инициализацией. Моделирование указанных характеристик реализовано в программе Burai 1.3, а также на сайте materialsproject.org, позволяющем генерировать CIF файлы. Выявлено, что на основе использования псевдопотенциалов было уменьшено количество электронов, а так же сократилась необходимая энергия отсечения, которая имела рещающее значение в расчетах на основе плоских волн. Полученные результаты являются фундаментальными и могут быть полезны при изучении нанокристаллов.

Ключевые слова:нанокристаллы KF и LiF, зонная структура, плотность состояний, полная энергия, компьютерное моделирование.

Annotation. The paper presents the results of computer modeling of the band structure of KF and LiF in various spatial groups at a temperature of 0 K. To reduce the computational time, pseudopotentials were used, which took into account only the electrons involved in the binding. All computationin this paper were performed using spin polarization on magnetic ions with high spin ferromagnetic initialization. Modeling of the characteristics is implemented in the Burai 1.3 program, as well as a site that allows you to generate CIF files materialsproject.org. It was found that the use of pseudopotentials reduced the number of electrons, as well as reduced the required cutoff energy, which had a rescheduling value in the calculations based on plane waves. The results obtained are fundamental and can be useful in the study of nanocrystals.

Key words: KF and LiF nanocrystals, band structure, density of states, total energy, computer simulation.

Introduction. Alkali halide crystals (AHC) – representatives of the class of ionic compounds – have a fairly simple crystalline and electronic structure. As a result, they convenient model systems for studying various crystalline defects. Many of the physical properties of AHCs are very sensitive to the presence of defects in these crystals, including those due to the presence of various impurities in the crystal. The effect of external influences on the crystal, in particular, heating, exposure to radiation of various wavelength ranges (from X-ray to infrared), and deformation, can significantly depend on the type and concentration of activator centers present in the crystal lattice [1-3].

Interest in research in the physics of AHCs is also associated with the expansion of their practical application. The possibility of using these crystals as media for recording and storing information, active materials of optical quantum amplifiers and generators, radiation sensors of various types makes it relevant to study the processes that occur in them under various influences.

The basic idea of using pseudopotentials instead of truepotentials for atoms is based on the fact that mainly valence electrons determine the chemical and physical properties of materials, and underlying electrons are most often chemically inert and canconsidered in the approximation of a frozen skeleton. Orbitals of the coreelectrons are located closer to the nucleus and experience strong oscillations, which would require expansion of the wave functions in too large a set of basis functions (plane waves) in solving Kohn Sham equations. The use of pseudopotential significantly reduces computational costs not only by reducing the amount orbitals, but mainly due to a decrease in the required basis sets.It should be noted that the pseudopotential method played a decisive role indevelopment of the plane wave method in the theory of the density functional inKohn-Shem approximation, which is the dominant approach in the DFT. All calculations were performed using pseudopotentials with an expanded projection wave (PAW).

In this work, the calculations were carried out under the following conditions 0 K and 0 atm, and spin polarization on magnetic ions with high-spin ferromagnetic initialization is used, in this case, the system can relax to a state where a low spin is observed during relaxation of the charge

density functional. In this work, we used the following parameters for all calculations, a grid of *k*-points on a scale of 1000 / total number of atoms in a cell. Monk horst-Pak method for selecting *k*-points and the tetrahedron method for integrating *k*-points. We also used the Pymatgen method, which can change the calculus default parameters, that is, when one method of integrating *k*-points is not suitable, the system switches to other integration parameters of all points. You can read more about this method in [4-6].

Description of the object and methods of research

Most properties of a physical system are determined by its valence electrons. It is assumed that the behavior of the wave functions of the internal of electrons does not change when the external chemical environment atom. The pseudopotential approach uses the idea of replacing core electrons and strong ionic potential by a weaker pseudopotential, which acts on many pseudo-wave functions and defines everything pronounced properties of valence electrons, including relativistic effects. Thus, the investigated system is replaced by a system consisting of pseudovalent electrons and pseudoions whose potential is outside the radius cutoff r_C coincides with the potential of the true ion, but inside this sphere it much weaker. The Schrödinger equation in this case is solved inside the sphereof radius r_C is much easier, because the desired wave function decomposes in much fewer basic functions. The following criteria are essential for choosing the mostoptimal pseudopotential:

1) the pseudo-wave function should not contain nodes. It's necessary to obtain a smooth pseudo-wave function;

2) charges concentrated inside a sphere with radius r_C, for bothwave functions must match;

3) the pseudo-wave function must be continuous and double differentiable;

4) the eigenvalues of both wave functions must be equal.

In this work, pseudopotentials constructed withusing the PAW method. Valence wave functions tend to have fast oscillations near ionic core. This situation is problematic because it requires many Fourier components for an accurate description of wave functions. One of ways to solve this problem is to use pseudopotentials, inwhich collective system consisting of nuclei and core electrons, described by effective potential. Then the Kohn-Shem equationsare solved only for valence electrons. Projection method attachedwaves (Projector augmented wave method, PAW) solves this problem bytransforming these rapidly oscillating wave functions into smoothwave functions that are more convenient for calculations. MethodPAW generalizes the method of ultra soft pseudopotentials (US-PP) and linearized augmentedplane-wave (LAPW) method. PAW is a full electron method in whichthe full wave function is divided into parts, each of which is described according to the ideology of the attached waves, which facilitates the transition between full-electron function and pseudo-wave.

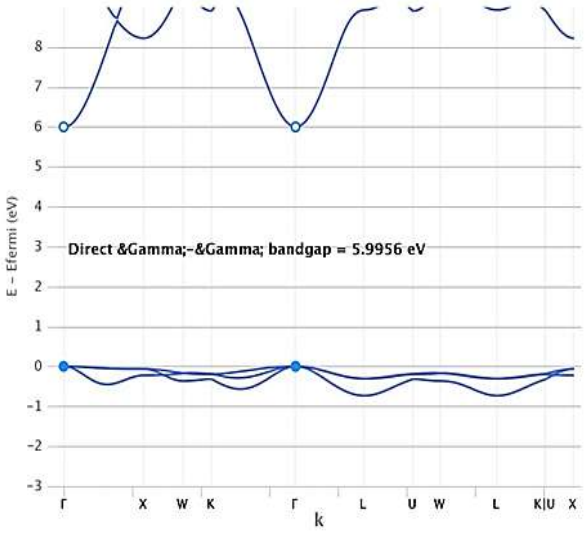
Simulation results. In general, forbidden zones calculated using common exchange-correlation functionals, such as LDA and GGA, are greatly underestimated. As a rule, in the literature, disagreement is about 50%. GGA accuracy is much higher than LDA, because the gradient is partially takes into account the non-locality of electronic interactions. Computational costshowever, they remain practically the same, since the dependence on the gradientintroduced into a predetermined value – exchange-correlation energy. By thisthe reason most modern DFT options are based on the approximation GGA.

The origin of the forbidden zone error and increase the accuracy. Errors in the forbidden zones of the DFT obtained from the calculations can be attributed to two sources:

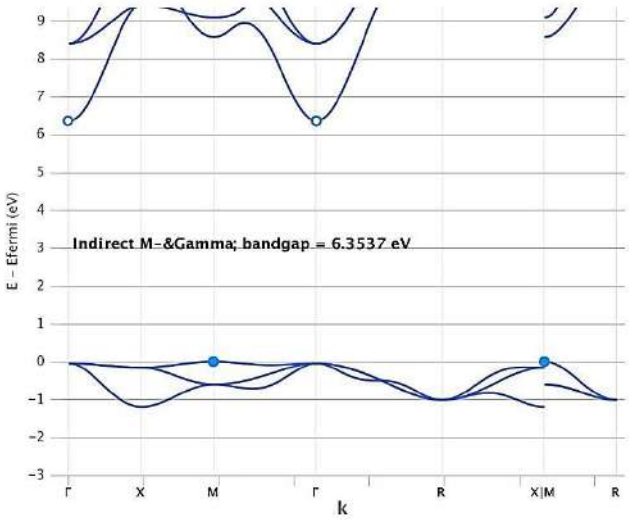
1. The approximations used for the exchange correlation functional.

2. The derivative term of discontinuity, originating from the true density functional, which is discontinuous with the total number of electrons in the system.

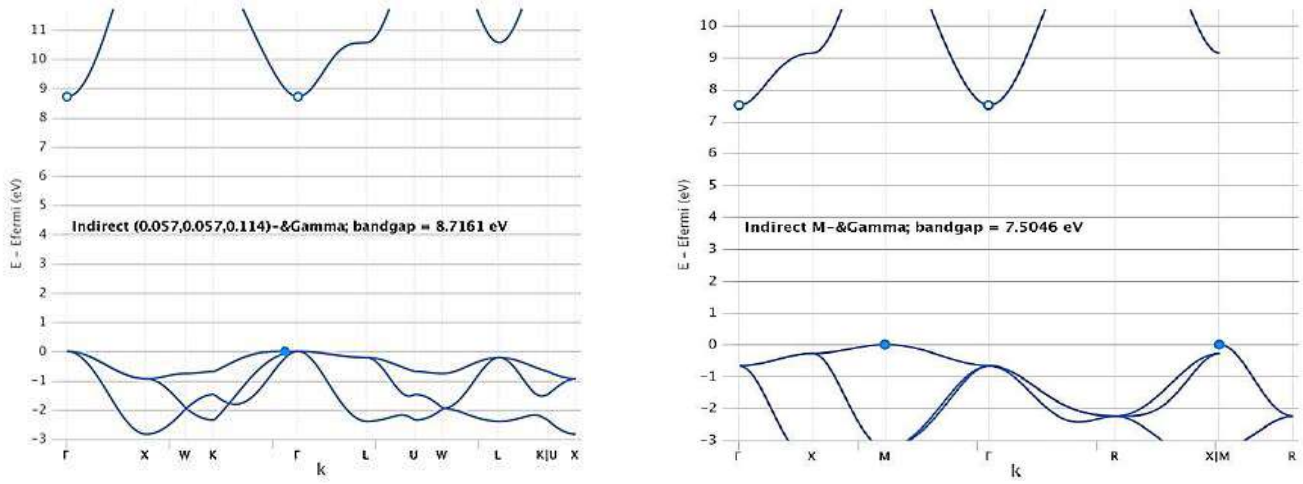
Also on the DFT results are influenced by the type of lattice which we took for payments in our calculations, we have 2 types of centered lattices is the *F* (*n* about superficially - centered) and P (centered on a certain side); calculation results are shown below (figure 1). For our calculations, we took two chemical compounds like KF and LiF. In this paper, we used the following pseudopotentials: K.pbe-spn-kjpaw_psl.1.0.0.UPF, F.pbe-n-kjpaw_psl.1.0.0.UPF,Li.pbe-s-kjpaw_psl.1.0.0.UPF



KF (surface centered)



KF (centered on a certain side)



LiF (surface centered) LiF (centered on a certain side)

Figure 1. Calculation results of KF and LiF nanocrystals

Of these contributions, (2) is usually considered a larger and more important contribution to the error. This can be partially solved using various methods, such as the GW approximation, but usually at high computational costs [7-8]. The table shows the band gap of KF and LiF nanocrystals.

Table. Band gap of KF and LiF nanocrystals

Nanocrystal	Band gap, eV		Experimental band gap, eV	Run Type
	P m_3m	F m_3m		
KF	6.3537	5.996	13.6	GGA
LiF	7.5046	8.736	10.7	

Conclusion. Thus, in this paper, the results of computer simulation of the band structure for different input parameters of the cell are presented, which strongly affect the calculation results. These calculations are fundamental for further research. Despite a wide variety of quantum-chemical methods, not one at present, letting you quantitatively describe the electronic system, and the accuracy depends on the choice of a package that has its pros and cons

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«ОПТИКАЛЫҚ АСПАПТАР» ТАҚЫРЫБЫНА АКТ ЖӘНЕ ДИАЛОГТЫҚ ОҚЫТУ ӘДІСТЕРІН ҚОЛДАНУ

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Қ.Жұбанов атындағы Ақтөбе өңірлік мемлекеттік университеті, Ақтөбе қаласы, Қазақстан

Аңдатпа. Мақалада жаңа инновациялық технологияларды пайдалана отырып, жан-жақты дамыған, көзі ашық, көкірегі ояу, қоғам үшін пайдасы зор жеке тұлға тәрбиелеуі жөнінде айтылған. Қоғам үшін білімді ұрпақ тәрбиелеуде мұғалімдер «дәстүрлі» әдістен бас тартып, жаңаша әдістер арқылы оқытуға көшуі туралы атап көрсетілген. Сонымен қатар оқушыларды өз-өздерін бағалай білуге, оқушылардың оқу ептілігін дамытуға, сындарлы ойлауға бағыттау керектігі аталып көрсетілген.

Түйін сөздер: инновациялық технологиялар, модуль, диалогтық оқыту, оптикалық аспаптар, АКТ.

Аннотация. В статье рассказывается о хорошо образованном, непредубежденном и образованном человеке с использованием новых инновационных технологий. Подчеркивается, что учителя в воспитании полезных для общества поколений отказались от «традиционного» метода и перешли на новые методы обучения. Это также подчеркивает необходимость самооценки, способности учеников к обучению и критического мышления.

Ключевые слова: инновационные технологии, модули, диалоги, оптические приборы, ИКТ.