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FINE STRUCTURE OF DIELECTRIC FUNCTION OF CADMIUM FLUORIDE

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Рассчитаны зоны, плотности состояний и спектры диэлектрической проницаемости с учетом и без учета матричных элементов переходов методом LAPW кристалла фторида кадмия. Результаты сопоставлены с ранее полученными методом FP-LMTO и рассчитанными на основе экспериментальных спектров отражения кривыми диэлектрической проницаемости. Установлены основные особенности оптических свойств фторида кадмия, границы применимости теоретических моделей, их достоинства и недостатки.

The electronic structure of solids has been extensively investigated for several decades within the density functional theory. The great success is achieved. However the many problems are appeared. One of them, the problem of correct calculation of the transition matrix elements, is very important to calculate the optical properties of crystals. In many papers the results are obtained without taking into account the probabilities of transitions. Recently, for the CdF₂ crystals we calculated the band structure, the densities of states $N(E)$, and the dielectric function $\epsilon_2(E)$ with the FP-LMTO method [1]. It seems to be more appropriate to say that we have determined the joint density of states because the probabilities of transitions are not taking into account. The goal of this work is the calculation of the ϵ_2 spectrum with and without taking into account the matrix elements within the LAPW method [2] and determine the influence of matrix elements on the optical properties of cadmium fluoride. Also we calculated the localizations of transitions in Brillouin zone (BZ).

Cadmium fluoride CdF₂ is a very promising in optoelectronic materials. The crystal CdF₂ is characterized with a large gap energy. It is a crystal structure the same the fluorite CaF₂. However the optical properties of two compounds are strongly distinguished due to the high-lying valence band originated from the 3d states of cation in the CdF₂; in the case of CaF₂, these states are formed the bottom of lowest conduction band (LCB). The band structure of cadmium fluoride is showed on fig.1. The energy gap E_g equals 3.9 eV. This is less than experimental data on ~ 4.2 eV. The top of highest valence band (HVB) has been set to zero of energy. The HVB consists from six subbands formed generally by 2p states of F⁻. But the contribution of the 3d states of Cd²⁺ is also large, especially in the highest

subband. The full width of HVB equals 3.4 eV. This is very well agreed with the experimental results [3]. The next five subbands are formed from the 3d states of the cadmium ion and lied about 0.9 eV below HVB. The location of these bands is overestimated by 0.8 eV as compared with the photoemission data [3]. The partial spectra of densities of states show the contributions of 2p states of F⁻ to the second valence band are significance (fig.2). More detail investigation of the band origin into whole volume of BZ shows that the occupied states of the anion and cation are comparatively strong mixed for the top of HVB (0 – 1 eV) and the bottom of second valence band (4.5 – 5.3 eV). The core band, almost fully formed by 2s states of fluorine, lies on about 20 eV below the top of HVB. The conduction bands structure is more complex. In the range 4 – 20 eV they are formed from the 4s states of cadmium and 3p states of fluorine. Generally, these results are very well agreed with our previous FP-LMTO data. The our theoretical results for the $\epsilon_2(E)$ spectra calculated with the LAPW method with (curve 1) and without (curve 2) taking into account the matrix elements of transitions, the FP-LMTO method without taking into account the matrix elements (curve 3), and the spectrum of ϵ_2 calculated in paper [4] on the base of experimental $R(E)$ spectrum of paper [3] (curve 4) are shown on fig.3. The curves 2 and 3 are shown in an arbitrary units and normalized on the maxima of theoretical curve 1.

The theoretical spectra 2 and 3 are well agreed between them in the 8–20 and 30 – 40 eV energy range. In the range 16 – 30 eV the structure of the spectra is due to transitions from the 3d valence bands to conduction bands. Hence, the discrepancies of two curves appear due to different methods to describe the localized states in LAPW and FP-LMTO methods.

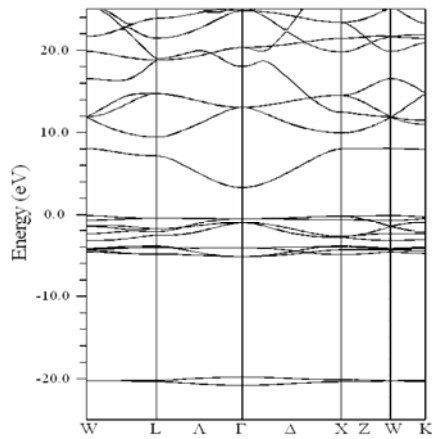


Fig. 1. The band structure of cadmium fluoride

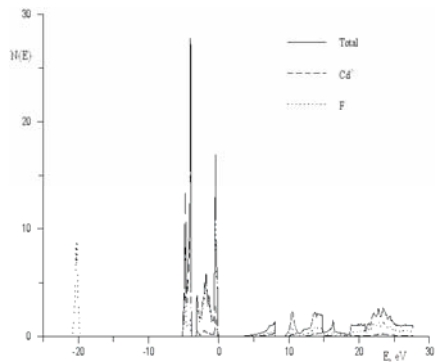


Fig. 2. The densities of states of cadmium fluoride

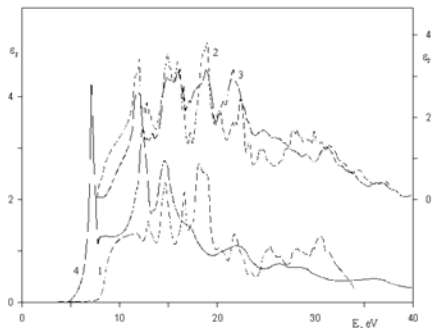


Fig. 3. The $\epsilon_2(E)$ spectra of cadmium fluoride, calculated theoretically with (1) and without (2, 3) accounting of the matrix elements within the LAPW (1, 2) and FP-LMTO (3) methods and from the experimental $R(E)$ spectra of paper [3] (4)

The significant changes are observed with taking into account the matrix elements. The theoretical spectrum 1 and calculated one 4 also strongly appreciate. The longest wavelength maximum of spectra 4 has an exciton nature and, of course, it is disappeared in the one-electron spectra 1 – 3. The second intensive peak with maximum at 10.3 eV (curve 4) is well obtained in the curve getting without the matrix elements, but it is a very small in spectrum 1. The third peak with the maximum at 15 eV is obtained in all theoretical spectra. However in the spectra 2 and 3, it is a very complex and wider than experimental-calculated one. But it is underestimated in the spectra 1. The analysis of the results shows that the second and third peaks may have an metastable exciton origin. At the higher energy range (17–20 eV) the very intensive wide peak is observed in the theoretical spectra. In the spectrum 4 it is absent. The three comparatively weak peaks of the spectra 4 in the 20 – 35 eV energy range have analogs in the spectrum 1. Therefore, the accounting of the matrix elements for the CdF₂ crystals improves the accordance of the theoretical results with the experimental-calculated data. However this agreement may be random due to obscurity of strong localized *d* states of cadmium.

Besides the integral spectra of $\epsilon_2(E)$, we calculated the localizations of optical transitions into the volume of BZ. Earlier we obtained that the optical transitions in CdF₂ are happened generally in the volume of BZ [1], but not at the points of symmetrical directions as it common accepted. The calculations with the accounting of the matrix elements are affirmed this conclusion. Moreover, the localizations for the most intensive transitions appearing in both spectra 1 and 2 are almost independent from the matrix elements.

So, in present work the new interesting information about the electronic structure of cadmium fluoride is obtained. It can be useful to discussion of the known physical and chemical properties of CdF₂.

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