Dispersion and Thin Spin-Depended Splittings of Electronic π-Bands in Transition Metal Dichalcogenide Crystals and Monolayers

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The dispersion of the electronic states of transition metal dichalcogenides crystals 2H-MeX_2 a (Me=Mo, W; X=S,Se,Te) s well as their monolayers has been investigated by using the symmetric theoretical group methods.
It is shown that the results of the developed methods of theoretical-group analysis are consistent with the data of experimental and computational studies of energy spectra and multiplicities of degeneration of quantum states of pi-electron zones.

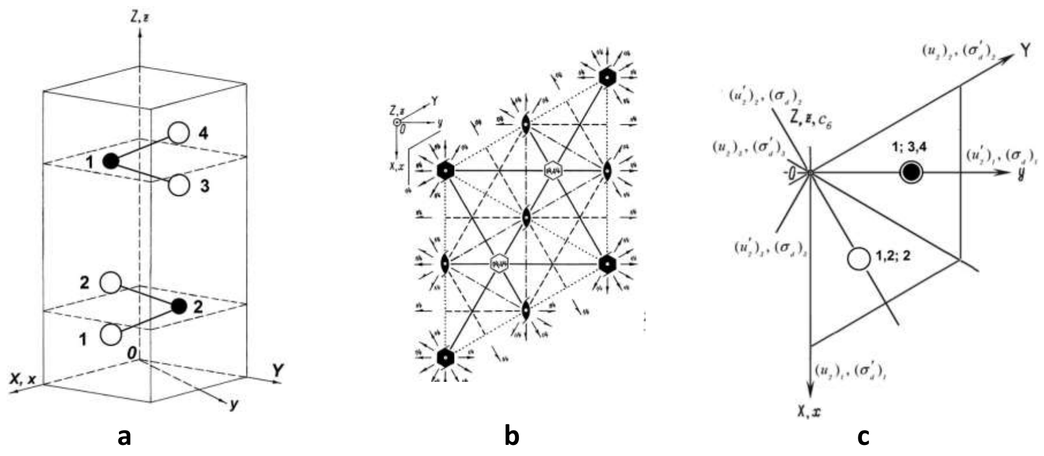


Figure 1. Structure of standard unit cell of hexagonal crystalline 2H-MeX_2 (a); t he standard diagramme of the spatial symmetry group P63 /mmc (D_{6h}^4) **(b)**; orientation of the elements of the point symmetry group 6/mmm (D_{6h}) **(c)**. The circles indicate the positions of the atoms of metal (dark) and halogen (transparent).

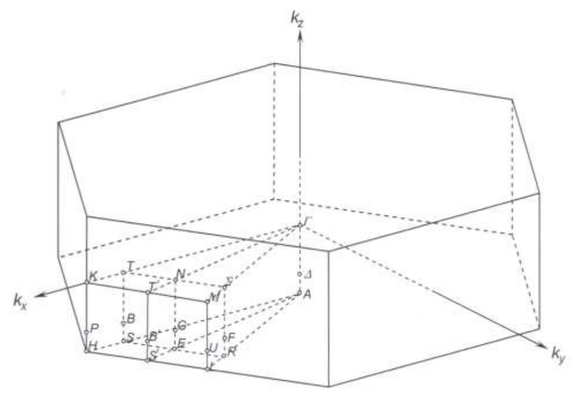


Figure 2. Brillouin zone of 2H-MeX_2 crystals and its symmetry points

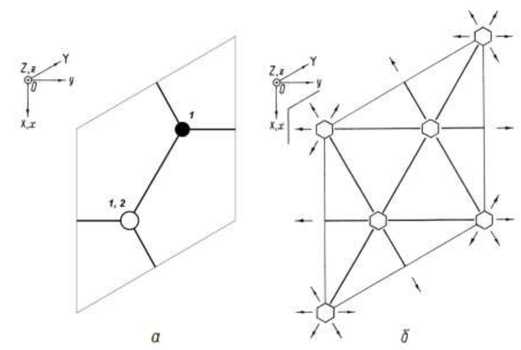
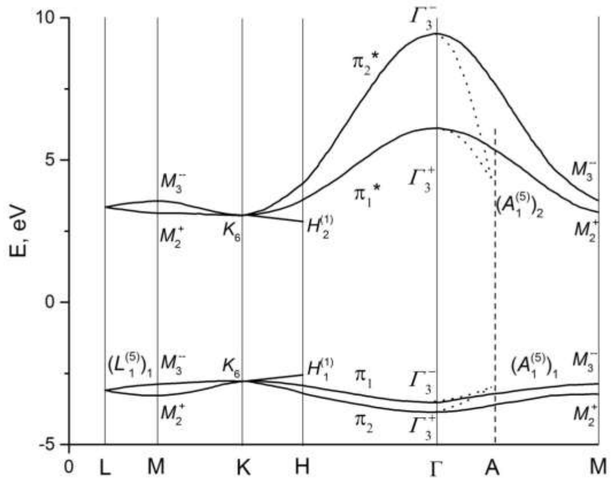


Figure 3. Structure of the standard unit cell of single-layer of 2H-MeX_2 **(a)**; the diagram of the spatial symmetry group DG78 **(b).**



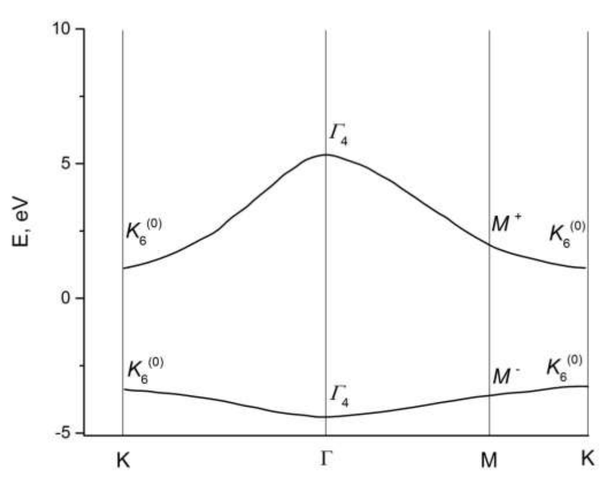


Figure 4. Dispersion of the electron energy π-bands in the 2H-MeX_2 crystal **(a)** and a single-layer (letters mark the points in the Brillouin zone, and indexed letters do the irreducible projective representations of the corresponding projective classes)

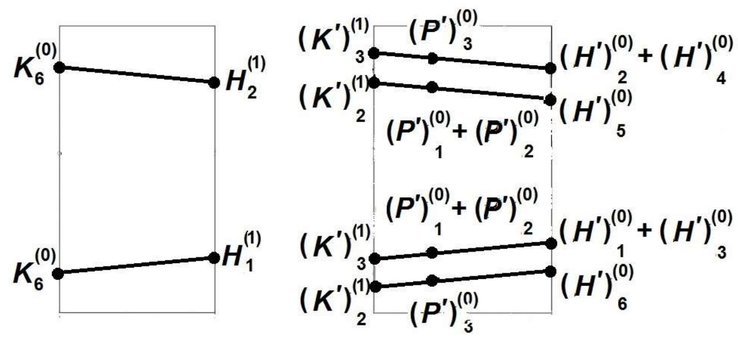


Figure 5 Dispersion of electronic energy π- and π *-bands in the Brillouin zone of hexagonal crystals of 2H_MeX_2 along the line $K-P-H$: without taking (a) and taking the electron spin into account (b)

Table 1 Irreducible projective representations of the K point of the MeX_2 monolayer

(C_{3h})	e	c_3	c_3^2	ic_2	ic_6^5	ic_6
$K_1^{(0)}$	1	1	1	1	1	1
$K_2^{(0)}$	1	1	1	−1	−1	−1
$K_3^{(0)}$	1	ϵ_3	ϵ_3^{-1}	1	ϵ_3	ϵ_3^{-1}
$K_4^{(0)}$	1	ϵ_3	ϵ_3^{-1}	−1	$-\epsilon_3$	$-\epsilon_3^{-1}$
$K_5^{(0)}$	1	ϵ_3^{-1}	ϵ_3	1	ϵ_3^{-1}	ϵ_3
$K_6^{(0)}$	1	ϵ_3^{-1}	ϵ_3	−1	$-\epsilon_3^{-1}$	$-\epsilon_3$

Table 2 Irreducible projective representations of the K point of the MeX_2(taking into account spine of electrone)

$\bar{6}\ (C_{3h})$	e	c_3	c_3^2	ic_2	ic_6^5	ic_6
$(K')_1^{(0)}$	1	−1	1	i	$-i$	$-i$
$(K')_2^{(0)}$	1	−1	1	$-i$	i	i
$(K')_3^{(0)}$	1	$-\epsilon_3$	ϵ_3^{-1}	i	ϵ_{12}	$-\epsilon_{12}^{-1}$
$(K')_4^{(0)}$	1	$-\epsilon_3$	ϵ_3^{-1}	$-i$	$-\epsilon_{12}$	ϵ_{12}^{-1}
$(K')_5^{(0)}$	1	$-\epsilon_3^{-1}$	ϵ_3	i	$-\epsilon_{12}^{-1}$	ϵ_{12}
$(K')_6^{(0)}$	1	$-\epsilon_3^{-1}$	ϵ_3	$-i$	ϵ_{12}^{-1}	$-\epsilon_{12}$

Table 3 Representation of electronic π-zones of the MeX_2 monolayer

$\bar{6}\ (C_{3h})$	e	c_3	c_3^2	ic_2	ic_6^5	ic_6
K_{eq}	2	−1	−1	2	−1	−1
K_z	1	1	1	−1	−1	−1
K_π	2	−1	−1	−2	1	1
$K_{\mathbf{r}}$	3	0	0	1	−2	−2
K_{vib}	6	0	0	2	2	2
$D_{1/2}^+$	2	1	−1	0	$-\sqrt{3}$	$\sqrt{3}$
K_z'	2	1	−1	0	$\sqrt{3}$	$-\sqrt{3}$
K_π'	4	−1	1	0	$-\sqrt{3}$	$\sqrt{3}$

The projective two-valued representations of spinor states for different points of Brollouin zones of crystalline 2H transition metal have been constructed for the first time.
Projective classes, which transform spin-dependent electronic wave functions at the points of high symmetry of the Brillouin zone have been determined for the above-mentioned structures. For the establishment of projective classes we found the method of constructing of factor systems, in particular, the correct factor system for spinor representations; the form of standard factor systems and the phase factors for their conversion to standard factor systems for each projective class have been found.