THEORY OF ABSORPTION SPECTRA OF MOLECULAR CRYSTALS

A.S. DAVYDOV

Institute of Physics, Academy of Sciences of the Ukrainian SSR
(Kyiv, Ukraine)

A general theory describing electron energy states in molecular crystals has been developed. The theory is used to elucidate some features of the absorption spectra of monoclinic crystals of the naphthalene and anthracene types. The shift of nondegenerate energy levels and their splitting into two components with different polarizations have been demonstrated to occur in crystals of these types.

1. Formulation of the Problem. Basic Formulas

From our point of view, while analyzing the optical properties of molecular crystals, the most convenient way is to proceed from a rough consideration of a crystal as an aggregation of individual molecules located in the lattice that is characteristic of the given crystal.

In the first approximation, we consider molecules to be rigidly fixed at their equilibrium positions and to be characterized by a certain spatial orientation (if the molecules are asymmetric). Thermal motion of molecules, as well as of atoms in them, which gives rise to the emergence of a rotational-vibrational structure, can be taken into account indirectly, similarly to what is done when molecular spectra are analyzed.

As known, we can always distinguish a group of electrons in molecules, whose energy states govern the molecular absorption in the far long-wave range of the spectrum and whose wave functions overlap weakly with the wave functions of other electrons. We refer to such electrons as "optical". For plenty of organic compounds, these are the so-called π-electrons.

Let us suppose that a crystal consists of identical molecules, and let each of them possess S "optical" electrons. The state of the k-th molecule is determined by the wave function depending on the coordinates and the spins of those electrons. Such a function can be presented as a product of a function depending only on the coordinates (ω_k) and a function depending only on

the spins (χ_k) of those electrons:

$$\varphi_k = \omega_k \chi_k.$$

Let H_k be the energy operator for the k-th molecule, and let V_{kn} be the energy operator describing the interaction between the k-th and n-th molecules. Then the wave functions and the energy levels (E) of stationary states in the whole crystal are determined by the Schrödinger equation

$$\left(\sum_k H_k + \sum_{k<l} V_{kl} - E \right) \Phi = 0. \tag{1}$$

Here, the summation is carried out over all N molecules in the crystal. The wave function Φ depends on the coordinates of all electrons[1]; the coordinates of molecules and their spatial orientations will be regarded as parameters. In what follows, the positions and orientations of molecules in the lattice will be designated by a single symbolic vector **R**.

While studying the problem of light absorption and emission by a crystal in the visible and ultraviolet spectral ranges, we are interested in the normal and the first excited states of the crystal. Let Φ_0 be the wave function of the crystal, provided that all its molecules are in the normal state. In the zero-order approximation, the wave function Φ_0 can be presented as an antisymmetrized product of the normal-state wave functions φ_i of individual molecules:

$$\Phi_0 = \frac{1}{\sqrt{(SN)!}} \sum_\nu (-1)^\nu P_\nu \psi, \tag{2}$$

where

$$\psi = \varphi_1 \varphi_2 \dots \varphi_N, \tag{3}$$

P_ν stands for one of $(SN)!$ possible permutations of electrons, and the summation is carried out over all

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[1] Since hereafter we deal with "optical" electrons only, the word "optical" is omitted.

possible permutations. All φ_i-functions are assumed normalized and real-valued. In addition, we neglect the integrals of nonorthogonality (overlapping) between the wave functions belonging to neighbor molecules.

In the first approximation, the energy of a crystal can be determined from Eq. (1). For this purpose, we substitute Eq. (2) into it, multiply the result by Eq. (3), and integrate the product over all coordinates of electrons:

$$E^0 = \sum_k E_k^0 + \sum_{k<l} \left\{ \int \varphi_k^2(\text{I}) V_{kl} \varphi_l^2(\text{II}) d\tau - \right.$$

$$\left. - \sum_\mu \int \varphi_k(\text{I}) \varphi_l(\text{II}) V_{kl} \varphi_k(\text{II}) \varphi_l(\text{I}) d\tau \right\}. \tag{4}$$

Here, $\varphi_k(\text{I})$ and $\varphi_l(\text{II})$ are the wave functions of molecules k and l for some arrangement of electrons in the molecules; $\varphi_k(\text{II})$ and $\varphi_l(\text{I})$ are the same functions, provided the permutation of a certain pair of electrons from molecules k and l; and the summation over μ includes all possible electron pair permutations between the k-th and l-th molecules.

Now, let

$$\psi_n = \varphi_1 \varphi_2 \ldots \varphi_n' \ldots \varphi_N \tag{5}$$

be the wave function of electrons, provided that the n-th molecule is in a nondegenerate excited state, and all the molecules are located at rather large distances from one another. If the molecules are brought closer to one another (until the crystal is formed), the excitation is no more localized at the n-th molecule, but it is transferred from one molecule to another one[2]. Therefore, the wave function of the excited crystal state antisymmetrized with respect to electron permutations can be approximately presented as a superposition of states

$$\phi_n = \frac{1}{\sqrt{(SN)!}} \sum_\nu (-1)^\nu P_\nu \psi_n \tag{6}$$

with definite amplitudes a_n depending on the coordinates $\mathbf{R}$ of all molecules:

$$\Phi = \frac{1}{\sqrt{N}} \sum_n a_n(\mathbf{R}) \phi_n, \tag{7}$$

[2]The transfer of the excitation from one molecule to another one is similar to the propagation of excitation waves in ionic and "atomic" lattices (a system of identical atoms located at sites of a spatial lattice with one electron per atom) considered by Frenkel [1] (Frenkel's excitons) and Peierls [2].

where the value of $|a_n(\mathbf{R})|^2$ corresponds to the probability of the event, when the n-th molecule turns out excited at a given arrangement of all molecules.

Substituting Eq. (7) into Eq. (1), multiplying the result by ψ_m, and integrating over the coordinates of all electrons, we obtain the system of algebraic equations to determine a_n and the crystal energy E:

$$\sum_n{}' a_n M_{mn} - \varepsilon a_m = 0 \quad (m = 1 \ldots N), \tag{8}$$

where the summation is performed over all the molecules except for the m-th one; the matrix element

$$M_{nm} = \int \varphi_m'(\text{I}) \varphi_n(\text{II}) V_{mn} \varphi_m(\text{I}) \varphi_n'(\text{II}) d\tau - $$

$$- \sum_\mu \int \varphi_m'(\text{I}) \varphi_n(\text{II}) V_{mn} \varphi_m(\text{II}) \varphi_n'(\text{I}) d\tau \tag{9}$$

characterizes the excitation exchange between the n-th and m-th molecules;

$$-\varepsilon = E_m' + \sum_k{}' \left\{ E_k^0 + \int \varphi_m'^2(\text{I}) V_{mk} \varphi_k^2(\text{II}) d\tau - \right.$$

$$\left. - \sum_\mu \int \varphi_m'(\text{I}) \varphi_k(\text{II}) V_{mk} \varphi_m'(\text{II}) \varphi_k(\text{I}) d\tau \right\} +$$

$$+ \sum_{k<l}{}' \left\{ \int \varphi_k^2(\text{I}) V_{kl} \varphi_l^2(\text{II}) d\tau - \right.$$

$$\left. - \sum_\mu \int \varphi_k(\text{I}) \varphi_l(\text{II}) V_{kl} \varphi_k(\text{II}) \varphi_l(\text{I}) d\tau \right\} - E, \tag{10}$$

and the primed sums mean that the summation is carried out over all the molecules but the m-th one.

Subtracting the normal state energy E_0 (Eq. (4)) from E determined by Eq. (10), we obtain the excitation energy of the crystal as

$$\Delta E = \Delta E_m + D + \varepsilon, \tag{11}$$

where $\Delta E_m = E_m' - E_m^0$ is the excitation energy for a molecule, and

$$D = \sum_k{}' \left\{ \int \varphi_m'^2(\text{I}) V_{mk} \varphi_k^2(\text{II}) d\tau - \right.$$

$$- \int \varphi_m^2(\text{I}) V_{km} \varphi_k^2(\text{II}) d\tau - $$

$$- \sum_\mu \left[\int \varphi_m'(\text{I}) \varphi_k(\text{II}) V_{mk} \varphi_m'(\text{II}) \varphi_k(\text{I}) d\tau - \right.$$

$$\left. \left. - \int \varphi_m(\text{I}) \varphi_k(\text{II}) V_{mk} \varphi_m(\text{II}) \varphi_k(\text{I}) d\tau \right] \right\}. \tag{12}$$

Hence, the excitation energy of the crystal differs from the excitation energy of a molecule by two terms, D and ε.

To calculate ε, it is necessary to solve the system of equations (8) homogeneous with respect to a_n. In the case of a perfect periodic arrangement of molecules, the coefficients a_n can differ from one another only by the phase, because any molecule can be found in the excited state with the same probability. Therefore as usual, we seek a solution of the system of equations (8) in the form

$$a_n = e^{i\mathbf{k}\mathbf{n}}, \tag{13}$$

where the radius-vector $\mathbf{n}$ characterizes the position of the center of the n-th molecule in the crystal, and $\mathbf{k}$ is the wave vector that describes the excitation wave in the crystal.

Substituting Eq. (13) in Eq. (8) and fixing the coordinate origin at the m-th molecule, we obtain

$$\varepsilon = \sum_{l=1}^{N-1} e^{i\mathbf{k}\mathbf{l}} M_{0l}, \tag{14}$$

where $\mathbf{l} = \mathbf{m} - \mathbf{n}$. As is evident from Eq. (14), each discrete characteristic value of the electron energy in an isolated molecule corresponds to a band of densely located characteristic values of the electron energy in the crystal. The width of this band is determined by the values of integrals M_{0l} which characterize the excitation energy transfer from the 0-th to the l-th molecule. For molecular crystals, these integrals are small even for neighbor molecules (of the order of 0.01 eV and smaller).

To calculate the matrix elements (9), we take advantage of the expansion of the classical interaction energy V_{nm} between two molecules in a power series in $1/r_{nm}$. Confining the expansion to the first term (i.e. taking only the dipole-dipole interaction into account), we obtain

$$V_{nm} = -\frac{e^2}{r_{nm}^3} \sum_{i,j} \left\{ 2z_{in}z_{jm} - x_{in}x_{jm} - y_{in}y_{jm} \right\}, \tag{15}$$

where x_{in}, y_{in}, z_{in} and x_{jm}, y_{jm}, z_{jm} are the coordinates of the i-th and j-th electrons in two molecules measured in the corresponding coordinate frames that are fixed at the centers of those molecules and oriented in such a way that the line, which passes through the centers of molecules, coincides with the z-axis of both frames.

Substituting Eq. (15) into Eq. (9), we convince ourselves immediately that, in the case of dipole transitions in molecules, only the first integral, which is responsible for the resonance interaction between two molecules, is of practical importance. In this approximation, we obtain the matrix element (9) in the form

$$M_{nm} = -\frac{e^2}{r_{nm}^3} \left| \int \varphi' \mathbf{r} \varphi d\tau \right|^2 \times$$

$$\times \left\{ 2\cos\theta_m^z \cos\theta_n^z - \cos\theta_m^x \cos\theta_n^x - \cos\theta_m^y \cos\theta_n^y \right\}, \tag{16}$$

where $e \int \varphi' \mathbf{r} \varphi d\tau$ is the matrix element of the electric moment vector which governs the quantum-mechanical transitions within a molecule; $\cos\theta_m^x, \cos\theta_n^x, \ldots$ are the cosines of angles between the vectors of electric moments in the m-th and n-th molecules, respectively, and the coordinate axes.

For the forbidden dipole transitions, $\int \varphi' \mathbf{r} \varphi d\tau = 0$. In this case, the interactions of higher orders (quadrupole-quadrupole one and so on) have to be taken into account in Eq. (9). The second term in Eq. (9) cannot be rejected now, because, in some cases, it turns out comparable with the first one by the order of magnitude.

2. Energy Terms of Molecular Crystals Belonging to a Monoclinic System

Let us apply the results obtained in Section 1 to molecular crystals of the anthracene, naphthalene, and other types which crystallize in the monoclinic prismatic system characterized by the C_{2h} spatial group of symmetry. The elementary cell of such crystals contains two molecules, whose arrangement and orientation are well studied.

In Fig. 1, the scheme of spatial arrangement of anthracene molecules according to Robertson's data [3] is given. The anthracene molecule is flat, and it is characterized by rhombic symmetry. In the crystal, molecules are arranged in the cleavage planes (the ab-plane) in such a way that the centers of molecules are located at the centers and in the corners of ab-faces. In this case, the face-centered and corner molecules have different spatial orientations.

Below, we take into account only the interaction between molecules that lie in the same cleavage plane of the crystal (the ab-plane), because the interaction forces between molecules located in different cleavage planes are small in comparison with those between molecules in the same cleavage plane. We introduce the basic vectors $\mathbf{a}$ and $\mathbf{b}$ in the cleavage plane of the crystal. Then, the position of an arbitrary molecule in the cleavage plane can be characterized by the vector

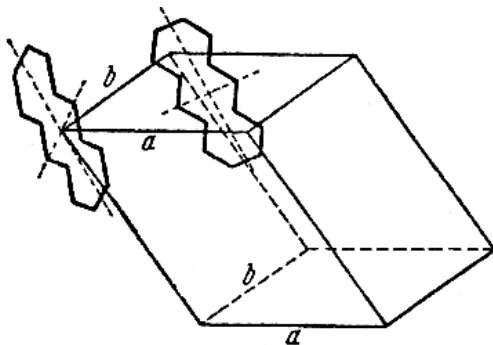$$\mathbf{l} = \frac{\mathbf{a}}{2} n + \frac{\mathbf{b}}{2} m, \tag{17}$$

Fig. 1

where the numbers n and m simultaneously accept either even or odd integer values, positive and negative. The molecules, the positions of which are characterized by even n and m, will be referred to as "even" molecules. The spatial orientations of all even molecules are identical (translation-equivalent molecules). The molecules, whose positions are characterized by odd n and m, will be referred to as "odd" ones. All odd molecules are translation-equivalent to one another, and their orientation is different from that of even molecules.

If the allowance is made for the excitation exchange only between neighbor molecules[3], then correction (14) of the molecular term can be written down in the form

$$\varepsilon = 2A\cos 2\eta + 2B\cos 2\xi + 4C\cos\eta\cos\xi, \quad (18)$$

where $\eta = \mathbf{kb}/2$, $\xi = \mathbf{ka}/2$, A is the matrix element (16) describing the interaction between two nearest – along the b-axis – molecules (both are either even or odd), B is the matrix element (16) describing the interaction between two nearest – along the a-axis – molecules (both are either even or odd), and C is the matrix element (16) describing the interaction between two nearest translation-inequivalent molecules (one even and one odd).

The wave function corresponding to energy (18) looks like

$$\Phi_{\xi\eta} = \frac{1}{\sqrt{N}}\sum_{n,m} e^{i(\xi n + \eta m)}\phi_{nm}, \quad (19)$$

where the summation is carried out over all even and odd values of n and m that characterize the position of molecules,

$$\phi_{nm} = \frac{1}{\sqrt{(SN)!}}\sum_{\nu}(-1)^{\nu}P_{\nu}\psi_{nm},$$

[3]Making allowance for the interaction at farther distances affects slightly the quantitative results and does not change the qualitative conclusions.

and

$$\psi_{nm} = \varphi_{11}\varphi_{22}\varphi_{13}\ldots\varphi'_{nm}\ldots.$$

To formulate the selection rules and to determine the polarization of additional transitions from the normal state Φ_0 into the excited one $\Phi_{\xi\eta}$ in the crystal, the matrix element

$$\mathbf{R} = \int \Phi_{\xi\eta}\mathbf{r}\Phi_0 d\tau, \quad (20)$$

where $\mathbf{r} = \sum_{n,m}\mathbf{r}_{nm}$, is to be calculated. By substituting functions (19) and (2) into Eq. (20), we convince ourselves that the matrix element (20) is zero for all ξ- and η-values, except for the cases 21

α) $\xi = \eta = 0$,

β) $\xi = 0$, $\eta = \pi$ (or $\xi = \pi$, $\eta = 0$). $\quad (21)$

Hence, the optical transitions (of the dipole type) in the crystal are allowed from the ground state into excited ones that are characterized by only two pairs of ξ- and η-values. Namely, the transitions are allowed into the states

$$\Phi_{\alpha} = \frac{1}{\sqrt{N}}\left\{\sum_{\text{even }n,m}\phi_{nm} + \sum_{\text{odd }n,m}\phi_{nm}\right\}, \quad (22)$$

$$\Phi_{\beta} = \frac{1}{\sqrt{N}}\left\{\sum_{\text{even }n,m}\phi_{nm} - \sum_{\text{odd }n,m}\phi_{nm}\right\}. \quad (23)$$

According to that, we obtain two types of the matrix elements (20): $\mathbf{R}_{\alpha}$ and $\mathbf{R}_{\beta}$. The transition with the matrix element $\mathbf{R}_{\alpha}$ different from zero is associated with the following variation of energy (11) in the crystal:

$$\Delta E_{\alpha} = \Delta E_m + D + 2A + 2B + 4C. \quad (24)$$

The transition characterized by the non-zero matrix element $\mathbf{R}_{\beta}$ is associated with the crystal energy variation

$$\Delta E_{\beta} = \Delta E_m + D + 2A + 2B - 4C. \quad (25)$$

As was shown by the author [4], the excited states of π-electrons in naphthalene molecules (the same is valid for anthracene ones as well) belonging to the D_{2h} point group of symmetry can belong to four irreducible representations A_{1g}, A_{2g}, B_{1u}, and B_{2u} of the D_{2h} symmetry group. The normal states of those molecules are related to the totally symmetric irreducible representation A_{1g}. The optical transitions from the

normal state are allowed only into the excited states B_{1u} and B_{2u} (with the polarization directed along the long and short axes of the molecule, respectively). The transitions into the states A_{1g} and A_{2g} are forbidden.

Knowing the symmetry of the wave functions, the selection rules, and the polarization of electron transitions in a molecule, one can to determine, making use of the group theory methods, the symmetric properties of the corresponding wave functions in a crystal and, as a consequence, to formulate the selection rules, as well as to find the polarization of the spectral lines for that crystal.

Of course, the character of the excited state of the crystal depends on the type of the relevant excited state of a molecule. Therefore, we denote the wave functions, which correspond to the excited state of the crystal, as $\Phi(\Gamma_l)$, where Γ_l will specify the character of the irreducible representation of the excited state of the molecule.

The characters of irreducible representations of the C_{2h} symmetry group of the crystal, as well as the transformation properties for the radius-vector components $(r_a, r_b, and r_{c'})$, are listed in the Table.

	E	C_2^b	i	σ^b	
A_g ...	1	1	1	1	
A_u ...	1	1	-1	-1	r_b
B_g ...	1	-1	1	-1	
B_u ...	1	-1	-1	1	$r_a, r_{c'}$

Note that the identical (E) and inversion (i) operations coincide both for a molecule and for the crystal. The operations of the crystal symmetry C_2^b and σ^b correspond to the permutation of "even" and "odd" molecules followed by either a rotation of the molecule by 180° around its short axis (operation C_2^y of the molecule) or the reflection of the molecule with respect to a plane perpendicular to that axis (operation σ^y of the molecule). Then, making use of the Table for the characters of irreducible representations of the molecular symmetry group, we obtain the following transformation properties for the wave function $\Phi_\alpha(B_{1u})$ of the crystal:

$$E\Phi_\alpha(B_{1u}) = \Phi_\alpha(B_{1u}), \quad C_2^b\Phi_\alpha(B_{1u}) = -\Phi_\alpha(B_{1u}),$$

$$i\Phi_\alpha(B_{1u}) = -\Phi_\alpha(B_{1u}), \quad \sigma^b\Phi_\alpha(B_{1u}) = \Phi_\alpha(B_{1u}).$$

Comparing the results obtained and the data in the Table of characters, one can see that the wave function $\Phi_\alpha(B_{1u})$ of the crystal is transformed similarly to the irreducible representation B_u of the C_{2h} symmetry group, which we write down shortly as

$$\Phi_\alpha(B_{1u}) \sim B_u.$$

In a similar way, we can determine the transformation properties for other functions:

$$\Phi_0(A_{1g}), \Phi_\alpha(A_{1g}), \Phi_\beta(A_{2g}) \sim A_g,$$

$$\Phi_\alpha(A_{2g}), \Phi_\beta(A_{1g}) \sim B_g,$$

$$\Phi_\alpha(B_{2u}), \Phi_\beta(B_{1u}) \sim A_u,$$

$$\Phi_\alpha(B_{1u}), \Phi_\beta(B_{2u}) \sim B_u.$$

Using group theory, we can now immediately formulate the selection rules and specify the polarization of the corresponding optical dipole transitions. All transitions from the normal state into the excited states of the crystal with the wave functions $\Phi_\alpha(A_{1g}), \Phi_\beta(A_{2g}), \Phi_\beta(A_{1g})$, and $\Phi_\beta(A_{2g})$ are forbidden. The transitions into all other levels are allowed. Hence, the transitions in the crystal are forbidden if they correspond to the forbidden transitions in the molecule and allowed if they correspond to the allowed transitions in the molecule.

Each allowed transition in the molecule corresponds to two allowed transitions in the crystal. In other words, the energy term of the molecule becomes split into two terms in the crystal, and those terms differ from each other by a polarization. One term is so polarized that its electric vector oscillates along the crystal b-axis, while the electric vector of the other term oscillates in the plane normal to the b-axis. The splitting of molecular terms is determined by different spatial orientations of anisotropic molecules in the crystal. If the molecules would have identical orientation, the splitting of the type studied here would have been absent, and only a shift of molecular terms would have been observed.

The magnitude of molecular term splitting is

$$\Delta = 8C. \tag{26}$$

The splitting of terms corresponding to forbidden transitions in the molecule is always smaller than the splitting of allowed terms.

The result obtained contradicts German's statement [8] that a possibility for the energy levels of a separate naphthalene molecule to be split in the naphthalene crystal can be excluded from consideration.

Both crystal terms are shifted with respect to the corresponding molecular term by the value of

$$\delta = D + 2A + 2B. \tag{27}$$

Both the shift amplitude and the splitting magnitude depend on the type of an electron transition in the molecule.

In this work, we have considered a modification of nondegenerate excited molecular states in a molecular crystal. If the molecule has degenerate excited levels, the degeneration can be removed if the molecule is placed into a crystal with a different symmetry. This will result in a splitting of molecular terms, similar to that of atomic terms, which has already been studied qualitatively in [6]. Every of the components that are split owing to the degeneration removal can be additionally split in the crystal due to the effect examined in this work.

A characteristic feature of molecular crystals is the fact that, at very low temperatures, the spectra of the crystal (both the absorption and fluorescence ones) consist of sharp and, often, very narrow bands. It was demonstrated in a series of works by I.V. Obreimow and A.F. Prikhotjko [7] devoted to studying the spectra of crystals at the liquid hydrogen temperature.

These spectra contradict seemingly the conventional ideas of the band structure of energy levels in crystals. Although the interaction forces in molecular crystals are small, the energy band width in such crystals should have been insignificantly different from the sublimation energy by the order of magnitude and should have reached hundreds of inverse centimeters. At the same time, the absorption spectrum of a naphthalene crystal includes so narrow bands [6] that some of them, by their width, remind emission lines.

As shown in this work, the discrete character of absorption lines is explained by the selection rules for optical transitions in the crystal, rather than by the narrowness of energy levels in it. The optical transitions are allowed only if the wave numbers acquire quite definite values.

In crystals of the anthracene or naphthalene types, the transitions can occur only between the ground level and the upper or lower edge of the energy band, provided that the crystal is in the excited state. Quantitative calculations of the absorption spectra of anthracene and naphthalene single crystals and the comparison of the results with experimental data will be carried out elsewhere.

In conclusion, I express my sincere gratitude to Prof. S.I. Pekar and Dr. A.F. Prikhotjko for the useful discussions and their interest in this study.

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DAVYDOV OLEKSANDR SERGIIOVYCH (26.12.1912–19.02.1993)

O.S. Davydov was the famous physicist-theoretician. He graduated from Moscow State University in 1939. From 1945 till 1953, O.S. Davydov worked at the Institute of Physics of the Acad. of Sci. of UkrSSR; in 1953–1956 – Head of a department at the Physico-Energetic Institute (Obninsk); 1956–1964 – Professor, Head of a chair of Moscow State University; 1964–1966 – Head of a department at the Institute of Physics of the Acad. of Sci. of UkrSSR; from 1966 – Head of a department at the Institute for Theoretical Physics of the Nat. Acad. of Sci. of Ukraine and, in 1973–1988, Director of this institute; Academician of the Acad. of Sci. of UkrSSR (1964); winner of the Lenin's prize (1966) and the State's prize of UkrSSR (1969); Honor Worker in Science and Technique of UkrSSR (1972); Hero of Socialist Labor (1982).

O.S. Davydov worked in the fields of solid-state physics, theory of nuclei, and theoretical biophysics. He was the first who expanded (1948) the notion of exciton to molecular crystals with complicated structure and indicated their decisive role in the processes of absorption of light, luminescence, and photoconduction. O.S. Davydov proved that even a small molecular interaction significantly changes, in the most cases, the energy spectrum of a real crystal and induces the splitting of nondegenerated molecular terms in crystals ("Davydov splitting"). He introduced (1951) the notion of deforming excitons and developed (1952) the theory of the impurity absorption of light by crystals; developed (1958–1960) the theory of collective excited states of nonspherical atomic nuclei with regard for the breaking of axial symmetry (the Davydov's theory of nonaxial nuclei); and constructed a model of contraction of muscles (1973–1976) within the theory of solitons. His main results are presented in the following monographs:

1. A.S. Davydov, *Theory of Light Absorption in Molecular Crystals* (Acad. Sci. of UkrSSR, Kiev, 1951) (in Russian).
2. A.S. Davydov, *Theory of Atomic Nuclei* (Fizmatgiz, Moscow, 1958) (in Russian).
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