

# Heavy doped organic crystals ordering

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The simple model that can describe structure and charge ordering in complex doped organic crystals is proposed. We consider the quasio-one-dimensional model of a crystal with chains (stacks) of flat BEDT-TTF molecules. In a chain of large molecules, small molecules fill every space between large molecules. The interaction between all molecules is described by the Lennard-Jones potential. It is shown that the small dopant molecules are in the double-well potential. It is shown that in case of the electrically neutral molecules at low temperatures there is a fluctuating structural ordering: the small molecules group in pairs near a large molecule, the lattice period in the fluctuation domain doubles. The structure of the boundary between the fluctuation domains is defined. In case of the charged molecules, correction to electric dipole interaction makes the system essentially three-dimensional, there is ferroelectric ordering in a chain and antiferroelectric one between the chains. Structure of the charge domains and domain boundaries are described.

Keywords: molecular crystal, quasio-one-dimensional model, dopants, charge ordering, domain boundaries.

## 1. Introduction

In organic crystals, charge ordering phase transitions occur in a limited temperature range below some critical temperature [1]. This kind of crystals has a complex character of internal interactions (see [2], Chap. 3). The most frequently studied organic crystals are BEDT-TTF (bis-ethylenedithio-tetrathiafulvalene). In such crystals, the charge ordering is possible by doping small molecules [3].

The BEDT-TTF molecules have shape of plate and interact mainly by wide molecular planes in the crystal [3]. The molecular planes are parallel to each other, and the molecules themselves form stacks with an axis perpendicular to the planes. It is easy to note that the system under consideration is similar to a strongly anisotropic layered crystal, in which the interactions inside the plane significantly exceed the interaction between the planes, which is described as a quasi-two-dimensional model [4]. The op-

posite case is also possible when the interaction within a chain of atoms (molecules) significantly exceeds the interaction between chains (quasi-one-dimensional model), like in liquid nematic crystals. Therefore, we will describe the BEDT-TTF crystal as a chain along the direction of molecular stacks. In this zero approximation we neglect the weak interaction between adjacent stacks (chains). In the first approximation we consider the interaction between the adjacent stacks (chains) that provides the crystal stability and 3D behavior in the phase transition description.

## 2. Quasi-1D model of organic crystal

We introduce a quai-1D model of the BEDT-TTF crystal, in which the chain consists of one molecular stack (Fig. 1) and the planes of the molecules are perpendicular to the direction of the one-dimensional chain. This assumption is consistent with the structural data of a real crystal [5].

The interactions between atoms can be clearly described by the Lennard-Jones potential expression [6], which has the following form:

$$U(r) = 4\varepsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right], \quad (1)$$

where  $\sigma$  is the finite distance at which the inter-particle potential is zero,  $\varepsilon$  is the depth of the potential well, and  $r$  is the distance between two particles. These parameters depend on the material. There is also another form of notation:

$$U(r) = \varepsilon \left[ \left( \frac{r_0}{r} \right)^{12} - 2 \left( \frac{r_0}{r} \right)^6 \right], \quad (2)$$

where  $r_0$  is the distance where the potential reaches its minimal value, i.e., an equilibrium distance. The interaction between the planes of large molecules (along the axis of the chain, Fig. 1) has a complex form like the Girifalco potential [7]. The formula for the Girifalco potential is similar to the Lennard-Jones one and includes sum of interactions between different atoms in neighboring molecules. We take a simplified averaged relation and use the formula (2) for intermolecular interaction along the chain.

In order to give conductive, super-conducting, magnetic, etc. properties to BEDT-TTF crystal and, thereby, expand its practical application, the small molecules are doped into the crystal. The role of the small molecules can play metal atoms or small organic molecules. We assume that these small molecules are located on the axis of the chain (stack). The interaction potential between large and small molecules (and small ones) can be written in a similar form:

$$U_s(r) = \varepsilon_s \left[ \left( \frac{r_s}{r} \right)^{12} - 2 \left( \frac{r_s}{r} \right)^6 \right], \quad (3)$$

$$U_{ss}(r) = \varepsilon_{ss} \left[ \left( \frac{r_{ss}}{r} \right)^{12} - 2 \left( \frac{r_{ss}}{r} \right)^6 \right],$$

where  $\varepsilon_s$  ( $\varepsilon_{ss}$ ) and  $r_s$  ( $r_{ss}$ ) are the depth of the potential well and the equilibrium distance large-small (small-small) molecules. The interactions of a small molecule with large one or two large molecules are shown in Fig. 2. We introduce the dimensionless variables:

$$x = \frac{r}{r_0}, \quad w = \frac{U}{\varepsilon}, \quad s = \frac{r_s}{r_0}, \quad s_s = \frac{r_{ss}}{r_0}. \quad (4)$$



Fig. 1. Quasione-dimensional (chain) model of the BEDT-TTF crystal. Bold vertical segments show projections along the large BEDT-TTF molecules.

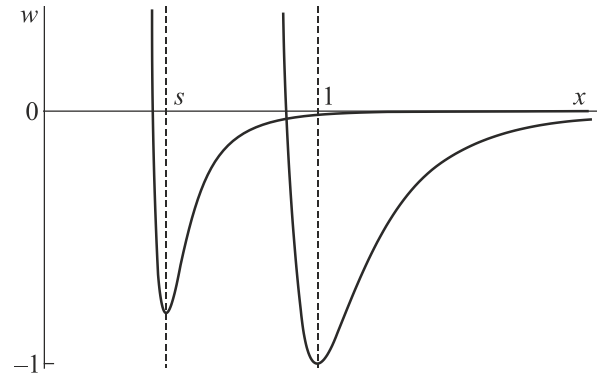


Fig. 2. Lennard-Jones potentials (2), (3) of interaction for the large (minimum in 1) and small (minimum in  $s$ ) molecules,  $\varepsilon_s = 0.8\varepsilon$ ,  $s = 0.45$ . Axes are displayed with non-dimensional units (4).

When  $r < r_0/2$ , a small molecule can be placed in a space between two large ones. For small molecules located between large molecules, the parameter  $s$  belongs to the range  $0 < s < 0.5$ . Otherwise, it is attracted to large molecules, but it cannot fill the space between them.

### 3. The double-well potential for a small dopant

The expression for the interaction potential of a small molecule with two large ones can be represented as the sum of interactions with each of two large molecules:

$$U_s(r) = \varepsilon_s \left[ \left( \frac{r_s}{r} \right)^{12} - 2 \left( \frac{r_s}{r} \right)^6 + \left( \frac{r_s}{r-r_0} \right)^{12} - 2 \left( \frac{r_s}{r-r_0} \right)^6 \right]. \quad (5)$$

Here it is assumed that the large molecules are located in the points “0” and  $r_0$  along the chain axes. In non-dimensional variables we obtain:

$$U_s(r) = \varepsilon_s \left[ \left( \frac{s}{x} \right)^{12} - 2 \left( \frac{s}{x} \right)^6 + \left( \frac{s}{x-1} \right)^{12} - 2 \left( \frac{s}{x-1} \right)^6 \right]. \quad (6)$$

The final form of the expression with a symmetric arrangement of large molecules relative to the  $w$  axis:

$$U_s(r) = \varepsilon_s \left[ \left( \frac{s}{x+0.5} \right)^{12} - 2 \left( \frac{s}{x+0.5} \right)^6 + \left( \frac{s}{x-0.5} \right)^{12} - 2 \left( \frac{s}{x-0.5} \right)^6 \right]. \quad (7)$$

Here we assume that the plain molecules are fixed in the points  $x = \pm 0.5$ . In the Fig. 3 (top panel) change in the space dependence of the potential (7) is shown for different values of the parameter  $s$ . The parameter  $s$  equals to the ratio of the equilibrium distances “large-small” and “large-large” molecules (3). For  $s < 0.45$ , the small molecule has the double-well potential [Figs. 3(a) and 3(b) (top panel)]. As the parameter  $s$  increases, the barrier width between wells for the small molecule decreases first [Fig. 3(b)], while the height of the barrier remains constant. Starting

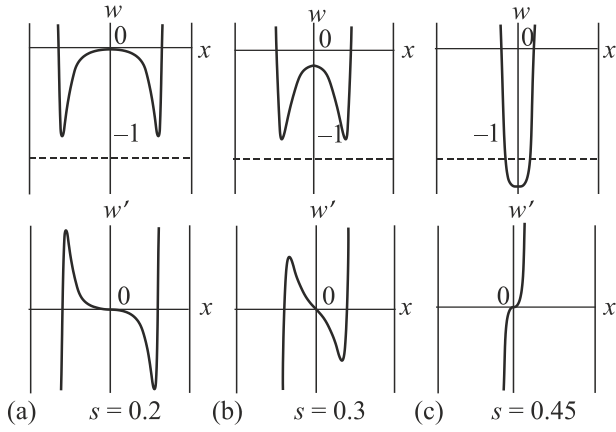


Fig. 3. For a small molecule the non-dimensional potential energy  $w(x)$  (top) and its space derivation  $w'(x)$  (bottom) dependences are shown for different values of the parameter  $s$ . The small molecule is located between two large molecules that are in points  $x = \pm 0.5$ . The bifurcation point (disappearance of the potential barrier in the well) is clearly observed at  $s = 0.45$  in  $w'(x)$  graph.

with  $s \approx 0.25$  [Fig. 3(b)], a decrease in the barrier height is observed, and with  $s = 0.45$  Fig. 3(c), the double well potential becomes a single well one (bifurcation point). Furthermore, we differentiate the expression (7) to obtain the function  $w'(r)$ , zeros of which correspond to the following extrema of  $w(r)$ : the middle extremum corresponds to the maximum, and two side ones correspond to the minima. Far from the bifurcation point, the side extrema are well described by the approximation  $r = r_s$  and  $r = r_0 - r_s$ , but this statement is not valid near the bifurcation point of the potential. The graph of the derivative  $w'(r)$  in Fig. 3 (bottom panel) allows us to clearly see the bifurcation point.

The height of the potential barrier in the double-well potential plays important role for the system behavior. The potential barrier height (see Fig. 4) can be found from expression:

$$h = U_{r_{\max}} - U_{r_{\min}}, \quad (8)$$

where  $U_{r_{\min}}$  is the potential in the minimum point and  $U_{r_{\max}}$  shows a potential value in the highest point [see Figs. 3(a) and 3(b)]. For small molecules, while  $0 \leq s \leq 0.25$ , the barrier height  $h$  is maximum and equals 1 when normalized to  $\epsilon$ . If  $s$  exceeds 0.45, the small molecule has one minimum of potential energy. If  $s$  exceeds 0.5, the small molecule cannot fill the space between large ones.

The following consideration we will start from the fact that each small dopant is in the double-well potential between the large molecules. Without any interaction between the small dopants, their potential energy is described by the formula (5) and energies in two wells of the double-well potential are equal. The set of the small dopants and the double-well potentials are shown in Fig. 5. Therefore, there is no ordering state of the small molecules. The aver-

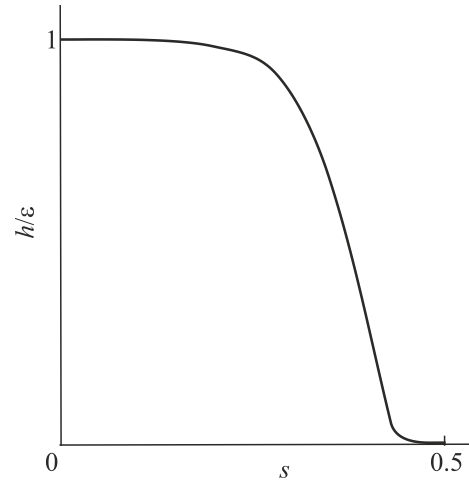


Fig. 4. The barrier height  $h/\epsilon$  of the double-well potential in dependence on the parameter  $s$ . The maximum of the barrier decreases starting from  $s \approx 0.25$  and disappears at  $s = 0.45$ .

age potentials of small molecules in disordered state have the same form in a high temperature phase.

The presence of the double-well potential consequently leads to an “order-disorder” phase transition [8, 9]. However the phase transition is impossible in one-dimension (chain) systems [8].

The average kinetic energy  $E_{\text{kin}} = 3kT/2$  of a small molecule is proportional to the temperature of the material. The ratio of this energy to the barrier height  $E_{\text{kin}}/h$  is the main parameter that determines the temperature  $T_{PT}$  when of the “order-disorder” phase transition can occur [1]. Due to the magnitude of  $E_{\text{kin}}/h = 1$ , the height of the barrier and  $T_{PT}$  are related:

$$h = \frac{3kT_{PT}}{2}. \quad (9)$$

At high temperatures  $T > T_{PT}$ , the small dopants move over the double-well potential barrier or easily jump between the wells. At low temperatures  $T < T_{PT}$ , the small molecules remain still in one of the two wells.

At low cooling rate, the system exists at  $T \approx T_{PT}$  for quite a long time, and the small dopants achieve the ordered state (see below). At high cooling rate, the system quickly passes the  $T_{PT}$  vicinity, and the relative weak interaction between the small molecules does not have time to arrange them.

We emphasize once again that relation (9) determines only the temperature below which the small molecules

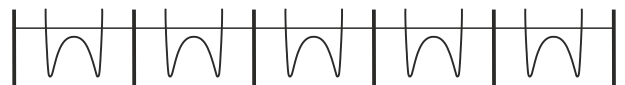


Fig. 5. Potentials of the small dopants without mutual interaction or in the high temperature disordered state. The large molecules are highlighted with bold vertical lines.  $s = 0.3$ .

remain in one of the two wells of the double-well potential. Then the “order-disorder” phase transition can occur only due to interaction between the small molecules. The phase transition is impossible and one-dimension systems are still disordered down to the temperature  $T = 0$  [8]. It is another matter that correlations grow with decreasing temperature, and the system is divided into domains, which the sizes grow with  $T$  decreasing.

Only accounting of interaction between the adjacent stacks (chains) provides the 3D behavior and correct the phase transition description.

#### 4. Interaction of neutral dopants and fluctuating domains

Let us consider two adjacent small unchanged dopant molecules, see Fig. 5, and fix position of one molecule. The distance  $r_1 = 2r_s = 2sr_0 < r_0$  corresponds to the nearest adjacent minima position of the small dopant molecules. The distance  $r_2 = r_0$  corresponds to periodic translation in the crystal. Therefore, in addition to the field of two neighboring large molecules (double-well potential for small dopant molecule) we will get the following interaction energy from the neighboring dopant:

$$U_{ss}(r_1) = \varepsilon_{ss} \left[ \left( \frac{r_{ss}}{r_1} \right)^{12} - 2 \left( \frac{r_{ss}}{r_1} \right)^6 \right] = \frac{\varepsilon_{ss}}{2^6} \left[ \frac{1}{2^6} - 2 \right], \quad r_1 = 2r_s,$$

$$U_{ss}(r_2) = \varepsilon_{ss} \left[ \left( \frac{r_{ss}}{r_2} \right)^{12} - 2 \left( \frac{r_{ss}}{r_2} \right)^6 \right] = \varepsilon_{ss} s_s^6 [s_s^6 - 2], \quad r_2 = r_0.$$
(10)

With any value of  $s < 0.5$  we obtain the following inequality

$$U_{ss}(r_1) < U_{ss}(r_2) < 0. \quad (11)$$

These values correspond to the minimum [ $U_{ss}(r_1)$ ] and maximum [ $U_{ss}(r_2)$ ] of the sloped double-well potential. In other words, two adjacent small dopant molecules attract and form pairs, the lattice period is doubled. The final local ordering of the neutral small molecules in a fluctuating domain is shown in Fig. 6(a). Due to the interaction of small molecules, every second large molecule attracts two nearest dopants. The model proposed here is a variation of the fully integrable one-dimensional Ising model, the complete solution of which was obtained by Ernst Ising [10].

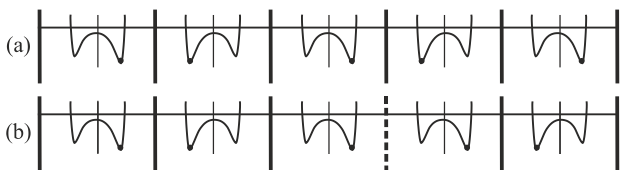


Fig. 6. (a) The potentials and arrangement of the small neutral molecules in a fluctuating domain. (b) The fluctuating domain boundary is shown as dashed line.

The proposed model is kind of the Ising model, in which the position of the dopant in the left and right wells corresponds to the up and down states. The considered interaction of the uncharged small dopants corresponds to the “antiferromagnetic” Ising chain.

A break of translational symmetry in the ordered state leads to the domain structure occurrence. Two adjacent domains display different positions of the small molecules and they are shifted at the lattice period, see Fig. 6(b). In the domain itself, the period is doubled. Approaching to the disordered state can be described as diminishing of the domains to a minimal size (a few periods).

It is obviously that the small dopant molecules interact very weakly between neighbor chains because of considerably long distances. So, 3D ordering of the small dopant molecules occurs at very low temperatures and by fluctuating way.

#### 5. The charge ordering and domains

In the case of different electronegativity of the small dopant molecule (may be metal atoms) and the large organic molecule, a charge transfer occurs. Then the molecules experience an electrostatic interaction. The Coulomb potential describes interaction of the small dopant molecules since their small size. The interaction between neighboring small molecules occurs in accordance with formula (6), taking into account the Coulomb potential. We introduce the notation for the electrostatic interaction of two large  $W_{LL}$  molecules and small and large  $W_{SL}$  molecules:

$$W_{LL} = \alpha \frac{q^2}{r}, \quad W_{SL} = -\beta \frac{q^2}{r}, \quad \alpha, \beta > 0, \quad (12)$$

where  $\alpha$  and  $\beta$  describe dependences on the large molecules shape, and  $r$  is distance between the molecules. Here, the different sign of the charges of the large and small molecules is taken into account. Let us find the change in the equilibrium distance between the large and small molecules introduced in (3), taking into account the electrostatic interaction  $W_{SL}$  in (12) as perturbation:

$$r_{sq} = r_s(1+b), \quad b = -\frac{\beta q^2}{72\varepsilon r_s} < 0. \quad (13)$$

Qualitatively similar result (shortening) can be obtained for another neighbor: distance small-large molecules increases. Therefore, the lattice period decreases, since the attraction of large and small molecules prevails over the repulsion of the charged molecules with the same charge. For the charged molecules we can obtain energies in the right and left well in dependence on position of neighboring charged small dopants [analogue of formula (10)]. We need to account that electrostatic interaction ( $\sim 1/R$ ) is long-range in comparison with Lennard-Jones attraction ( $\sim 1/R^6$ ). So, electrostatic interaction needs summation all over crystal and finding the Madelung sum (see [2], Chap. 3).

Different configurations of the small dopants are possible, but the most stable their arrangement (ordering) is shown in Fig. 7(a). This arrangement requires the most possible distance between the small dopants. All dopants are located in the left (or right) wells of the double-well potentials. The Madelung sum calculation is necessary to find exact values of the lattice period.

The proposed model is kind of the one-dimensional Ising model [10]. Here the position of the dopant in the left and right wells corresponds to the up and down states. The Coulomb interaction of the charged small dopants corresponds to the case of “ferromagnetic” Ising chain. Above we discussed that 1D systems can have only fluctuating ordering down to  $T = 0$ . The electrostatic potential provides enough strong interaction between the molecular chains (stacks) in the doped crystal. In this case the pairs of the oppositely charged molecules we can consider as electric dipoles with easy axis along a chain. Inside a chain the parallel arrangement of dipoles provides minimal energy [11]. In [Fig. 7(a)] all dopants can also be located in the right wells of the double-well potential, and then there is another domain in the charge ordered structure in the chain. The crystal with charged molecules can have a polycrystalline structure. In a chain the domain boundaries between charged ordered domains are shown in [Figs. 7(b) and 7(c)]. All dopants can be shifted away from the boundary [Fig. 7(b)], but they can approach to the boundary [Fig. 7(c)]. Electrostatic energies of these domain boundaries are different. Thus, in the chain we have different electrostatic interaction energies per one pair of neighboring dopant atoms:

$$W_a = \frac{q^2}{r_0}, W_b = \frac{q^2}{2r_0(1-s)}, W_c = \frac{q^2}{2r_0s}, \quad (14)$$

$$W_c > W_a > W_b.$$

Here  $W_a, W_b, W_c$  are the interaction energies per one pair inside a domain [Fig. 7(a)], and in the boundaries [Figs. 7(b) and 7(c)] correspondingly. Despite the fact that the energy  $W_b$  in the domain boundary [Fig. 7(b)] is the lowest, the number of such boundaries  $n_b$  is determined

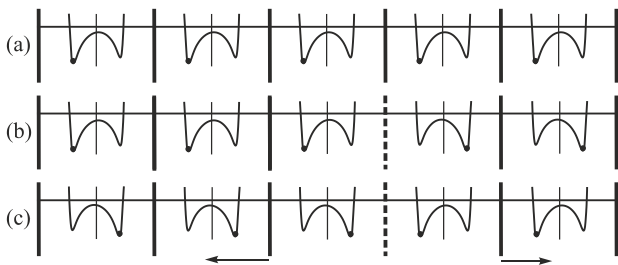


Fig. 7. (a) Charge ordering state in a chain. One (left) of possible two domains is shown. (b), (c) Domains and domain boundaries in the crystal with the charge-ordered small dopant molecules. (b) The left-right boundary; (c) the right-left boundary, the arrows show the electric dipoles orientations in the domains.

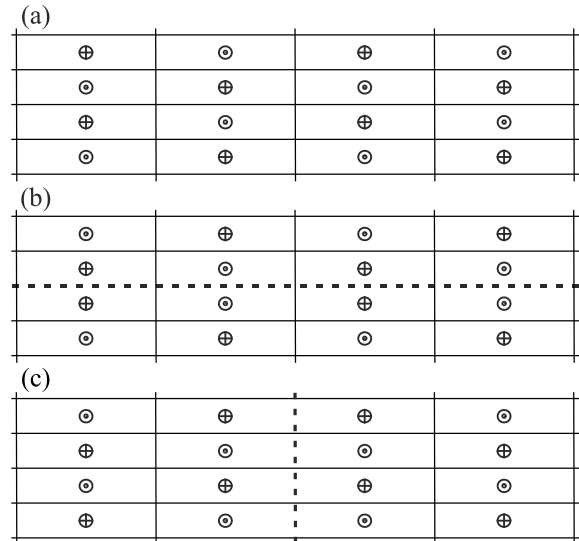


Fig. 8. (a) Transverse cross-section (chess packaging) of the parallel chains (stacks) in the charge ordered crystal. The rectangles correspond to the BEDT-TTF molecules with real size proportion [3]. The dipoles orientation is shown by up ( $\odot$ ) and down ( $\oplus$ ) vectors. (b), (c) The domain boundaries in the chess packaging.

only together with the number of the boundaries [Fig. 7(c)] due to their topological nature  $n_b = n_c \pm 1$ . Evaluations (14) seem to be more correct in comparison with dipole-dipole interaction because of small distances between dipoles in a boundary along a chain.

In the nearest neighboring chains, the axes of dipoles are perpendicular to the dipole-dipole line. In this case the dipoles arrangement is antiparallel [11]. Therefore, the chess packaging [Fig. 8(a)] of the dipoles in parallel chains (stacks) provide stability to the 3D charge ordering under “order-disorder” phase transition [8, 9]. The lattice period is doubled in both directions perpendicular to the chains. This perfect chess packaging structure [Fig. 8(a)] can be formed at slow cooling. Nucleation of the domains is independent that causes wrong in the chess packaging translation. Two kinds of the formed domain walls in the chess packaging structure are shown in Figs. 8(b) and 8(c).

Considered above the perfect chess packaging domain structure is formed at relatively slow crystal cooling. At high cooling rate multiple domain nucleations leads to the very short charge domains in the chains and very small chess-packaging domains. Annealing causes to coagulation of the domains in the chains and in the chess packaging simultaneously.

### 6. Conclusion

The organic crystals of TTF type exhibit various specific behaviors due to their structure and physical properties in dependence of the temperature. To provide new properties of organic crystals and, therefore, expand their practical application, dopants are inserted into the structure of the TTF crystal. In this paper, we considered the case of the



small dopants as interstitial impurity. Initially a model of a homogeneous quasi-one-dimensional crystal (chain) was considered; next, the same model, but with dopant molecules was described. We represented the interaction of the molecules by the Lennard-Jones potential. The existence of interstitial dopants is possible only when the dopant radius is much smaller than the TTF large molecule. In any other conditions, the dopant cannot fit between large molecules and should be located between TTF stacks. To describe the possibilities of doping the crystal, we introduced the parameter  $s = r_s / r_0$  for the ratio of the equilibrium distance between large and small molecules to the equilibrium distance between large molecules. It was shown that arrangement of a dopant inside the chain is possible only with the values of the parameter  $s < 0.5$ . In the chains for  $s < 0.45$ , the potential of a small dopant molecule becomes double-well (bifurcation). For the small dopants the condition of the double-well potential existence was considered. It was found that for the small dopant molecules the potential barrier increases with decreasing of the parameter  $s$ . For a more accurate and visual analysis, we use the potential's derivative which is more sensitive to the confluence of the potential extremes. It is shown that the small dopants ordering in the double-well potentials is possible only by taking into account interactions with neighboring dopants second neighbors.

In the case of the small neutral dopant molecules attraction, the double-well potentials become asymmetric, the small dopants are located in pairs, and the lattice period doubles. Because of very weak interaction of the dopant, the chain (stack) system is essentially one-dimensional. Consequently, phase transition and ordering have fluctuating character till  $T = 0$ .

In the case of different electronegativity of the large and small molecules, the charge transfer takes place between the molecules. Electrostatic interaction becomes the molecular chains into essentially three-dimensional system; therefore, the charge ordering phase transition is possible. It is shown that inside the molecular chain the ferroelectric ordering of the molecular dipoles has minimal energy and two possible domain boundaries structure in the chains is pointed out. It is shown that the antiferroelectric chess packaging ordering of the molecular chains dipoles exists in the plane perpendicular to the chains. Two domain boundaries can exist in chess packaging.

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#### Впорядкування сильно легованих органічних кристалів

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Запропоновано просту модель, яка може описати структуру та зарядове впорядкування у складних допованих органічних кристалах. Розглянуто квазіодновимірну модель кристала з ланцюжками (стопками) плоских молекул BEDT-TTF. У ланцюжку великих молекул малі молекули заповнюють кожен проміжок між великими молекулами. Взаємодія всіх молекул визначається потенціалом Леннард-Джонса. Показано, що малі молекули допанта розміщені у двоявному потенціалі. У випадку електронейтральних молекул, при низьких температурах відбувається флуктуаційне структурне впорядкування: малі молекули групуються в пари біля великих молекул, період ґратки у флуктуаційному домені подвоюється. Визначено структуру границі між флуктуаційними доменами. У випадку заряджених молекул корекція на електричну взаємодію диполів робить систему суттєво тривимірною, відбувається сегнетоелектричне впорядкування в ланцюжку і антисегнетоелектричне між ланцюжками. Описано структуру можливих зарядових доменів та границь.

Ключові слова: молекулярний кристал, квазіодновимірна модель, допанти, зарядове впорядкування, доменні границі.