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Auxetic, Partially Auxetic, and Nonauxetic Behaviour in 2D Crystals of Hard Cyclic Tetramers

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Poisson's ratios of 2D crystals of hard, cyclic tetramers, further referred to as *tetramers*, are investigated by Monte Carlo (MC) simulations. The tetramers, very simple model molecules, which are composed of four identical hard disks of diameter σ with centers forming a square of side d, are studied in the isobaric–isothermal ensemble. It is found that, at the same thermodynamical parameters, but depending on the anisotropy parameter $\alpha = d/\sigma$, the tetramers spontaneously form crystalline phases, representing each of the five Bravais lattices (BLs) which are possible in the 2D space. The following BLs are observed: 1) the oblique (monoclinic) one, 2) the rectangular (orthorhombic) one, 3) the centered rectangular (orthorhombic) one, 4) the hexagonal one, and 5) the square (tetragonal) one. Among them, structures showing auxetic, partially auxetic, and nonauxetic behaviour are found. This fact makes the tetramer an interesting example of a prototype "molecule," which, depending on its shape, assembles materials of all possible behaviors regarding Poisson's ratio. It is worth noting that tetramers with $\alpha = 1.7$ form a strongly auxetic phase that, at the considered thermodynamic conditions, reaches Poisson's ratios varying in the range between $-0.589(3)$ and $-0.162(4)$.

The development of nanotechnology leads to more possibilities of obtaining nanostructures with any requested geometry.[1–3] The latter, together with the intermolecular interactions, has a decisive influence on properties of the obtained material. In particular, if a crystal structure is formed, its symmetry has a crucial impact on its elastic properties. An important question is the one on the direct impact of a particle shape, size, and the interaction potential on the elastic properties of the system that such particles form. For a better understanding of the elastic properties of materials and for predicting new physical phenomena, which may find applications in future, one can use fairly simple model systems. It is known that 2D materials[4,5] and simple model systems[6,7] can exhibit unusual elastic properties, like auxeticity. Auxetic systems[8–12] show negative Poisson's ratio (NPR). The Poisson's ratio describes the ratio of the change of a transverse dimension of the system to the change of its longitudinal dimension under an infinitesimal change of longitudinal stress.[13] NPR indicates a rather nonintuitive behaviour of the material. It is manifested by a decrease in the transverse dimensions of the system under compression and by an increase in its transverse dimensions under tension. After the early works of Almgren,[14] Kolpakov,[15] Lakes,[16] Wojciechowski,[6,17] Evans et al.,[18] and Milton,[19] one can observe a great increase of interest in auxetic systems,[20–23] which translates into the intensification of the research aimed at searching for auxetic materials[24–27] and models exhibiting auxetic behaviour.[28–35] One can classify auxetic materials and models as follows. Materials with a positive Poisson's ratio are called *nonauxetic*. The *auxetic* systems have an NPR regardless of the direction of applied stress and the direction of its measurement. In the case in which the value of Poisson's ratio is negative in some directions and positive in other ones, one deals with a *partial auxetic*.[36] For example, majority of metals with body-centered cubic structures are partial auxetics as they show NPRs in some crystallographic directions and positive Poisson's ratios in others.[9] One should add that since the first mention of systems with an NPR, various manmade auxetic and partially auxetic materials have been produced, e.g., polyurethane foams,[16] composites,[37] and other structures based on a model of rotating squares.[38]

In this work, we analyze the impact of the geometry of very simple model "molecules" on the Poisson's ratio of the crystalline phases they form. We consider systems of *hard cyclic tetramers*, further referred to as *tetramers*, which are composed of four identical hard disks of diameters σ with centers forming a square of side d. The ratio $\alpha = d/\sigma$ defines the anisotropy parameter of a tetramer, see **Figure 1**a. Systems of such molecules, for the anisotropy parameter $\alpha = 1$, were studied using both mechanical simulations[39] and computer simulations.[40] Those studies showed a rich phase diagram[39] and auxetic properties of one of its crystalline phases.[40]

Remark: In this work, we do not take into account the well-known problems with the long-range translational order in 2D.[41]

It is known that in 2D the crystal structures can have one of five Bravais lattices (BLs)[42] that belong to four crystal families: monoclinic, orthorhombic, tetragonal, and hexagonal. These are lattices such as oblique, rectangular, centered rectangular, hexagonal, and square. Until now, hexagonal, rectangular, and square

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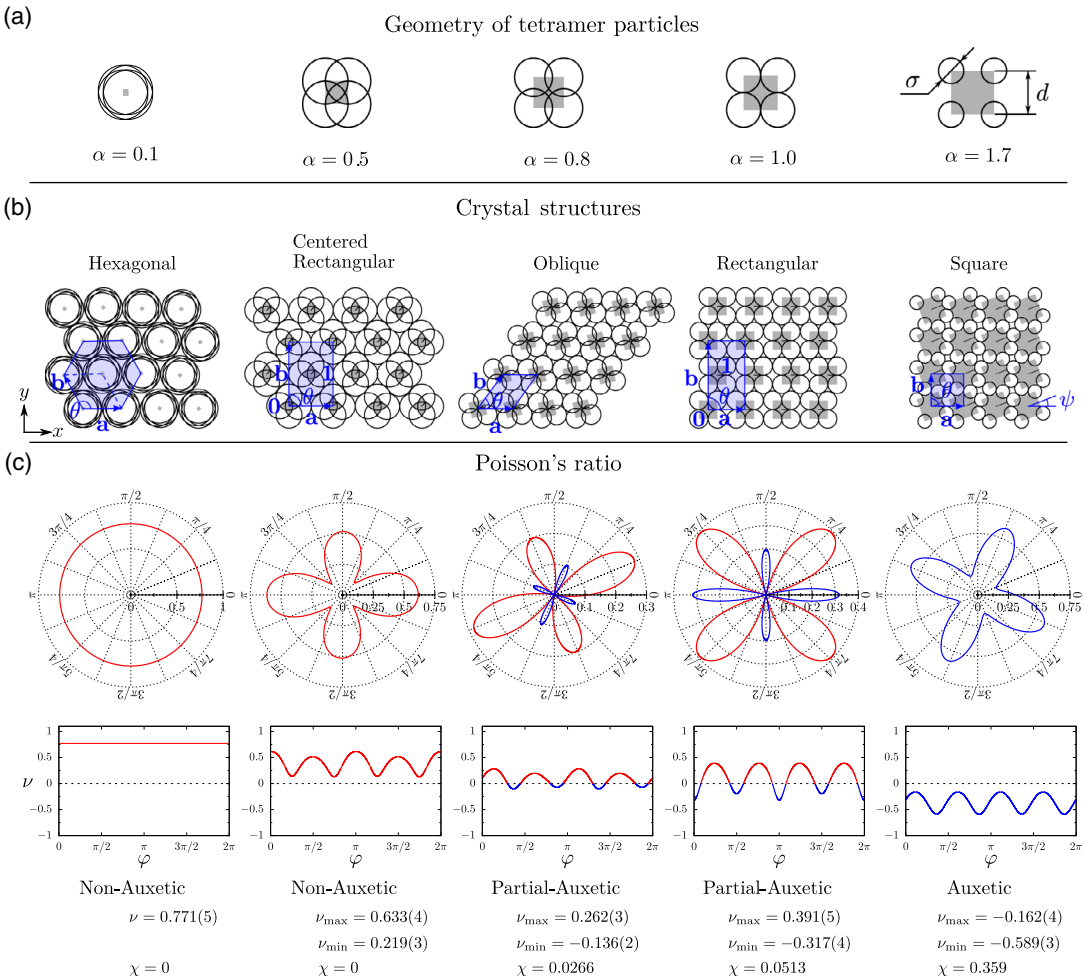

Figure 1. a) The geometry of tetramers with various anisotropy parameters. b) Structures of the tetramer systems with corresponding BLs. The unit cells are denoted by dashed/blue lines and their parameters are shown in Table 1. c) Orientational dependencies of the Poisson's ratio in the studied 2D systems are represented both in the polar coordinate system and in the Cartesian coordinate system. The positive and negative values of the Poisson's ratio are plotted in red and blue colour, respectively.

lattices have been observed for hard cyclic tetramers.[39] The aim of this work is twofold. First, we show that tetramers with a different anisotropy parameter, α, can form crystallographic structures with all five BLs at the same thermodynamic parameters. Second, we present the Poisson's ratio behaviour for these crystals and show that the studied crystals of tetramers exhibit the auxetic, partially auxetic, and nonauxetic properties. We also provide analytic formulas for Poisson's ratio for all crystal families in the 2D space.

The tetramer, see Figure 1a, is a nonconvex, hard-body model molecule of fourfold symmetry axis perpendicular to the molecular plane. In the model system under consideration, tetramers interact with each other through the hard potential which is equal to infinity when the tetramers overlap and zero otherwise. Five systems composed of tetramers with different anisotropy parameters, α, were considered. Computer simulations reveal that, at the same thermodynamic conditions, tetramers with different anisotropies ($\alpha = 0.1, 0.5, 0.8, 1.0, 1.7$) form spontaneously 2D crystals with all five BLs, see Figure 1b. The simulations of tetramers for the square and rectangular BLs were conducted for systems consisting of $N = 256$ tetramers. For the oblique lattice, $N = 196$ particles were used, whereas $N = 144$ were used for the centered rectangular and hexagonal lattices. Such numbers of particles are based on the results of previous studies. Namely, as it has been shown in earlier works[40,43–45] on hard cyclic multimers, simulations of systems of even less than 100 particles give results that differ by only a few percent from the results obtained by extrapolation to the limit $N \to \infty$. To calculate Poisson's ratio of the studied 2D crystals, the Monte Carlo (MC) simulations in the isobaric–isothermal ensemble with a variable box shape were performed. The elastic compliances have been calculated by the Parrinello–Rahman method[46–48] which is based on the analysis of the fluctuations of the strain tensor components at equilibrium. $S_{ijkl} = \langle \varepsilon_{ij} \varepsilon_{kl} \rangle \frac{V_p}{k_B T}$, where ε_{ij} is the strain tensor, V_p is the volume of the equilibrium state at pressure p, k_B is the Boltzmann constant, T is the temperature, and $\langle \dots \rangle$ are the averages in the isothermal–isobaric

ensemble.[43] More details on the method can be found in our earlier work.[43] The typical length of the runs was 10^7 trial steps per tetramer (cycles) for all sizes of systems, and 10% of the simulation length was considered as the equilibration time and was not taken into account in the calculation of the Poisson's ratio.

In this work, the Voigt notation[49] has been used where the indices 1, 2, and 3 denote xx, yy, and xy, respectively. It is required to take into account an appropriate coefficient between the elastic compliances in the tensorial form and the Voigt notation: $S_{11} = S_{xxxx}$, $S_{22} = S_{yyyy}$, $S_{12} = S_{xxyy}$, $S_{13} = 2S_{xxxy}$, $S_{23} = 2S_{xyyy}$, and $S_{33} = 4S_{xyxy}$. Later, we consider examples of the crystal families which one can distinguish in 2D.

The analytic expression for Poisson's ratio in the *monoclinic system* reads[45]

$$\nu(\varphi) = \left(1 + 4\frac{S_{11} + 2S_{12} + S_{22} + (S_{11} - S_{22})\cos 2\varphi + (S_{13} + S_{23})\sin 2\varphi}{-S_{11} - 6S_{12} - S_{22} + S_{33} + (S_{11} - 2S_{12} + S_{22} - S_{33})\cos 4\varphi + 2(S_{13} - S_{23})\sin 4\varphi}\right)^{-1} \tag{1}$$

As $S_{13} = S_{23} = 0$ in the *orthorhombic system*, the above formula for rectangular lattices simplifies to

$$\nu(\varphi) = -\frac{S_{11} + 6S_{12} + S_{22} - S_{33} - (S_{11} - 2S_{12} + S_{22} - S_{33})\cos 4\varphi}{8(S_{11}\cos^4\varphi + (2S_{12} + S_{33})\cos^2\varphi\sin^2\varphi + S_{22}\sin^4\varphi)} \tag{2}$$

In the *tetragonal system*, in addition to the previous changes, it should be taken into account that $S_{22} = S_{11}$. Therefore the Poisson's ratio for a square lattice, in the case of a primitive cell (with one atom per unit cell),[42] can be simplified to the form

$$\nu(\varphi) = 1 - \frac{8(S_{11} + S_{12})}{8S_{11} + (2S_{11} - 2S_{12} - S_{33})(\cos 4\varphi - 1)} \tag{3}$$

However, in the case of the one studied in this paper tetramer system, we have a 2D *chiral* square crystal. It is formed by adding a basis to every lattice point of the square BL. The basis contains one tetramer where the orientation does not match the orientations of the crystal axes. As a consequence, the mirror (reflection) symmetry of the x, y axes is lost and one gets $S_{23} = -S_{12}$ instead both being zero. The Poisson's ratio of the chiral square crystal can be written as

$$\nu(\varphi) = \left(1 + \frac{8(S_{11} + S_{12}) + 4(S_{13} - S_{12})\sin 2\varphi}{-2S_{11} - 6S_{12} + S_{33} + (2S_{11} - 2S_{12} - S_{33})\cos 4\varphi + 2(S_{12} + S_{13})\sin 4\varphi}\right)^{-1} \tag{4}$$

To describe the elastic properties of the *hexagonal system*, one needs only two elastic moduli. Taking into account that $S_{33} = 2(S_{11} - S_{12})$, one can see that Poisson's ratio for the hexagonal lattice is independent of the direction of measurement and can be written as

$$\nu = -\frac{S_{12}}{S_{11}} \tag{5}$$

The Poisson's ratio of a *perfect* auxetic in all directions is $\nu_{\text{perfect}} = -1$. Thus, in a polar coordinate system, a perfect auxetic can be represented by a circle of the unit radius $r_{\text{perfect}} = |\nu_{\text{perfect}}| = |-1| = 1$ and area $A_{\text{perfect}} = \pi$. In the case of the studied 2D systems, one can calculate the area of the negative part of the orientational dependence of the Poisson's ratio. This area, A, can be used to determine the radius r_s from the relation $A = \pi r_s^2$. The ratio of the radii r_s and r_{perfect} can be thought of as the *degree of auxeticity* for a given system.[50]

$$\chi = \frac{r_s}{r_{\text{perfect}}} = \frac{1}{2\pi}\int_0^{\pi}(|\nu(\varphi)| - \nu(\varphi))\mathrm{d}\varphi \tag{6}$$

Remark: The above definition is meaningful if there is no singularity in the orientational dependence of Poisson's ratio.

The Poisson's ratio of tetramer systems with different parameters of anisotropy was evaluated for the dimensionless pressure $p^* = p\sigma^2/(k_B T) = 100$. The choice of this pressure and particle anisotropy parameters was not accidental. At this pressure, the tetramers of the selected five anisotropy parameters form different crystals, representing each of the five BLs in 2D. Figure 1b shows the structures of tetramer systems that correspond to the following BLs: 1) tetramers with $\alpha = 1.7$ have a square lattice, 2) with $\alpha = 1.0$, we observe a rectangular lattice, 3) with $\alpha = 0.8$, we have an oblique lattice, 4) at $\alpha = 0.5$, we observe a centered rectangular lattice, and 5) tetramers with $\alpha = 0.1$ form a hexagonal lattice. The parameters of these crystal structures are shown in **Table 1**. It is worth noting that four of the presented structures have their equivalents at dense packing. In contrast, the structure with a hexagonal lattice occurs only in the rotational phase, i.e., when the tetramers have enough space to rotate almost freely. In the latter phase, the tetramers with $\alpha = 0.1$ can rotate around their centres. In the rotational phase, the tetramer system with $\alpha = 0.1$ behaves as a system isotropic for elastic properties. Figure 1c shows the Poisson's ratio of this system, both in the polar and in Cartesian coordinate systems. It is shown that Poisson's ratio does not depend on the direction of the measurement and is equal to 0.771(5). So, this system is clearly nonauxetic.

Remark: In 2D, the upper limit for the Poisson's ratio of an isotropic systems is +1, which is in contrast to 3D systems where it is equal to +0.5.[51]

An increase in anisotropy parameter to $\alpha = 0.5$, while maintaining the same thermodynamic parameters, leads to a change in the crystal structure of the system, which becomes a centered

Table 1. Parameters of the unit cells of the studied structures. The primitive basis of both rectangular structures has two tetramers at coordinates (x_0, y_0) and (x_1, y_1) associated with each point of the rectangular lattice, as shown in Figure 1b. The tetramer denoted by 0 is placed in the origin of the coordinate system (i.e. $x_0 = 0$ and $y_0 = 0$). x_1 and y_1 are coordinates of the center of the tetramer denoted by 1, as shown in Figure 1b. The basis of the rest of the structures contains only one tetramer. Figure 1b shows the definitions of parameters of the unit cells: a, b, ψ, and θ. All distances are given in units of σ. CP indicates close-packed structure.

Oblique (CP)			
$\lvert a\rvert = 1.7625$	$\lvert b\rvert = 2.1254$	$\psi = 0.2289$	$\theta = 0.9441$
Rectangular (CP)			
$\lvert a\rvert = 2.0$	$\lvert b\rvert = 3.732$	$\psi = 0$	$\theta = \pi/2$
$x_1 = \lvert a\rvert/4$	$y_1 = \lvert b\rvert/2$	$\psi = 0$	–
Centered rectangular (CP)			
$\lvert a\rvert = 1.7071$	$\lvert b\rvert = 2.439$	$\psi = \pi/4$	$\theta = \pi/2$
$x_1 = \lvert a\rvert/2$	$y_1 = \lvert b\rvert/2$	$\psi = \pi/4$	–
Square (CP)			
$\lvert a\rvert = 2.3835$	$\lvert b\rvert = \lvert a\rvert$	$\psi = 0.3646$	$\theta = \pi/2$
Hexagonal ($p^* = 100$)			
$\lvert a\rvert = 1.1390$	$\lvert b\rvert = \lvert a\rvert$	–	$\theta = 2\pi/3$

rectangular lattice, see Figure 1b. In this case, Poisson's ratio is direction dependent, whereas its value in all directions remains positive, as shown in Figure 1c. So, the system remains nonauxetic. The minimum value of Poisson's ratio is 0.152(3), and its maximum value is 0.633(4). One observes also different values of Poisson's ratio in the main crystallographic directions ($\nu_x = 0.219(3)$ and $\nu_y = 0.252(4)$).

For tetramers with the $\alpha = 0.8$, one gets a structure with the lowest symmetry among 2D crystals—the monoclinic system with an oblique BL. This structure has strongly anisotropic elastic properties, which are described by six elastic compliances. It is worth noting, however, that the tetramer's fourfold symmetry axis imposes its imprint on Poisson's ratio. Despite the low symmetry of the system, four crystallographic directions can be distinguished with two pairs of minima and two pairs of maxima in dependence of Poisson's ratio on the measurement direction. The values of both minima are negative ($\nu_{\min 1} = -0.136(3)$ an $\nu_{\min 2} = -0.100(2)$), whereas the maxima are positive ($\nu_{\max 1} = 0.262(3)$ and $\nu_{\max 2} = 0.176(3)$), which indicate that this system is partially auxetic, as shown in Figure 1c. The degree of auxeticity of this system, χ, is 0.0266. This result can be interpreted as indicating that this system is of only about 2.66% auxetic when compared with the perfect auxetic system ($\chi = 1.0$).

Previous studies have revealed the partial auxeticity of tetramers with the anisotropy parameter $\alpha = 1.0$ in the square structure.[40] However, the free volume theory[39] and recent extensive computer simulations indicate that tetramers with this anisotropy spontaneously crystallize into a rectangular structure, as shown in Figure 1b, which has the same density at close packing as the square (chiral) structure.[39] The Poisson's ratios in the main crystallographic directions have negative values, namely $\nu_x = -0.317(4)$ and $\nu_y = -0.196(3)$, but their values are larger than those observed for the square structure of tetramers with $\alpha = 1.0$ ($\nu_x = \nu_y = -0.345(3)$[40]). It is shown in Figure 1b,c that this rectangular lattice is partially auxetic with the degree of auxeticity close to 0.0513.

The last, fifth type of the tetramer, considered in this work, had the anisotropy $\alpha = 1.7$. Such particles spontaneously crystallize into a square lattice with the parameters shown in Table 1. Undoubtedly, the complete auxeticity of this system deserves special attention. Increasing the anisotropy parameter leads to stronger jamming between tetramers and their better mutual matching, which enhances the auxetic properties. As shown in Figure 1c, Poisson's ratio of the tetramer system with $\alpha = 1.7$ is negative in all crystallographic directions. In this case, the Poisson's ratio depends on the direction of measurement and, according to the symmetry of the crystal lattice, it is the same in the main crystallographic directions ($\nu_x = \nu_y = -0.309(4)$). The maximum value of the Poisson's ratio is $-0.162(4)$, its minimum value is $-0.589(3)$, and the computed degree of auxeticity is $\chi = 0.359$. This strongly auxetic system shows almost 36% of perfect auxeticity.

In summary, five model tetramer systems with various anisotropy parameters of particles, in which the tetramers interact through hard interactions, have been considered. Poisson's ratio of all the studied systems was determined by the MC version of the Parrinello–Rahman method.[43,46] The obtained results show that by changing the anisotropy of the tetramers, even at the same thermodynamic parameters, one can obtain crystals of all possible crystal lattices, which represent all BLs possible in 2D. Within this simple model, we found that, depending on the anisotropy parameter, the tetramer systems can present auxetic, partially auxetic, and nonauxetic behaviour, at the same thermodynamical parameters. Furthermore, strong auxetic properties were observed, in the system of tetramers with $\alpha = 1.7$, with a minimum value of Poisson's ratio reaching $-0.589(3)$.

A variety of crystal structures and their elastic properties, especially auxetic, make the tetramer an attractive model system. Taking into account the great possibilities of modern nanotechnology in the synthesis of nanoparticles and nanostructures of various geometries,[1–3,52–54] the results of this work may help in indicating the direction of the search and synthesis of interesting (quasi)2D auxetic materials.

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Conflict of Interest

The authors declare no conflict of interest.

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