

## Exotic shapes of nano-spherical structures - new DNA coding

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(joint work with Hassan Babiker)

The simplest naturally ordered tetrahedral packing consists of an ordered sequence of regular tetrahedra glued together face to face as with the linear packing of a tetrahedral helix. Such tetrahedral structures are called *tetrahedral chains*.

Any tetrahedral chain consists of the three types of simplest configurations of four consecutive tetrahedra called *tetrahedral units*. Two of these types are left and right tetrahedral short spirals,  $U, D$ , and the third type,  $F$ , is a flat configuration of four tetrahedra. The structure of a tetrahedral chain in  $D, F, U$  elementary units is written as a word like  $UUDFUD\dots$

The three strands of the left or right oriented tetrahedral helix form a spiral with irrational slope. This is the reason for the effective density of tetrahedral chains and nonexistence of closed tetrahedral chains in Euclidean space.

Let us assume that the gluing process of tetrahedra is ordered along a chain and each step of this process is realized by reflection in a particular face of adjacent tetrahedron. To each tetrahedron we assign four reflections  $R_i, i = 1, \dots, 4$ , in the configurational three dimensional space  $V$ . Reflections  $R_i$  in  $V$  are represented by four corresponding reflect-morphisms  $\bar{R}_i, i = 1, \dots, 4$ , acting in the space of regular tetrahedra  $\mathcal{T}$  through a reflectional transformation of their vertices. In  $V, \dim V = n$ , any tetrahedral chain of length  $n + 1$  is uniquely represented by an initial tetrahedron  $T$  and an ordered sequence of  $n$  reflect-morphisms

$$\bar{R}_{i_1}, \dots, \bar{R}_{i_n}, \quad i_k \neq i_{k+1}, k = 1, \dots, n-1.$$

The fact that a tetrahedral chain is so rigid in 3-space and regular tetrahedra can not tile the space gives rise to several questions. The main question we consider is the recognition of combinatorial and algebraic structures of tetrahedral chains. We want to investigate their geometric properties and determine what kind of information is contained in the chain invariants of orthogonal transformations and re-numberings. We use the parametrization of the chains by sequences of ordered reflections in barycentric coordinates and find their combinatorial structure. Periodicity along a chain is based on the structure of sequences of admissible triplets of integers and their cycling properties. The corresponding numerical invariants and an indexing role of a binary tetrahedral group defines the complete coding properties in dimension three.

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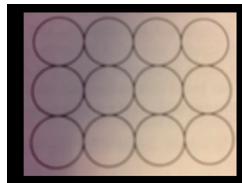
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## Sphere packings

- Square packing, face-centered cubic packing



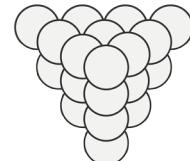
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- Barlow boy's packing, cell is a rhombic dodecahedron

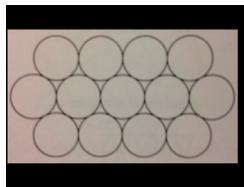


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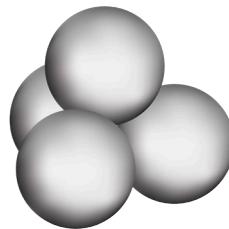
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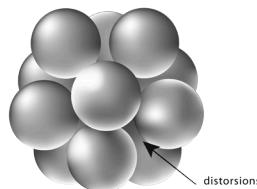


- Hexagonal packing, the third layer sits exactly above the first layer.

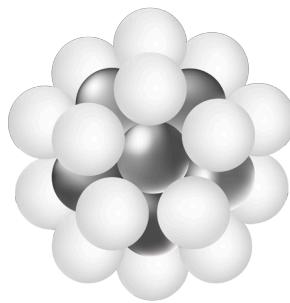
## Sphere packing



## Sphere packing



## Sphere packing

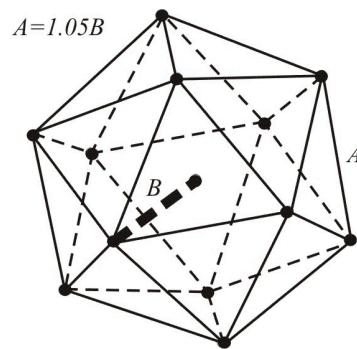


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## Icosahedron

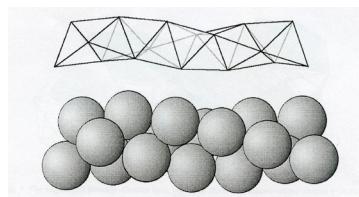


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## Tetrahedral chains



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## Tetrahedral chains



H. Steinhaus, 1957; J.H. Mason, 1972

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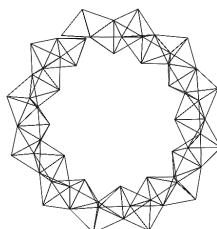
## Tetrahedral chains



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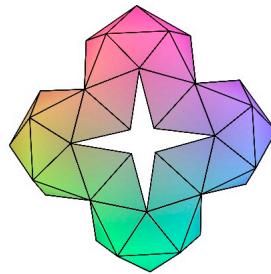
## Tetrahedral chains



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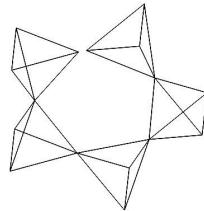
## Almost closed tetrahedral chains



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## Dual tetrahedral chains



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## Tetrahedra in barycentric coordinates

$$T \equiv \{p_1, p_2, p_3, p_4\}, \{(S_1, p_1), \dots, (S_4, p_4)\}$$

$\mathcal{T}$ -regular tetrahedra,  $\|p_i - p_j\| = \|p_k - p_l\|, i \neq j, k \neq l$

$$\mathcal{T} \subset V \otimes U^*, \quad U \equiv \mathbb{R}^4$$

$V$  - configurational affine space,  $\dim V = 3$

$U$  - barycentric coordinates  $(\alpha_1, \dots, \alpha_4) \in U$

$H = \{\sum_{i=1}^4 \alpha_i = 1\}$  - canonical affine hyperplane

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$$T \in \mathcal{T}, T = \sum_{i=1}^4 p_i \otimes e_i^*$$

**Barycentric coordinate map**  $\mathbb{T} : H \rightarrow V$ :

$$\mathbb{T}(\alpha) = \sum_{i=1}^4 p_i \otimes e_i^*(\alpha) = \sum_{i=1}^4 \alpha_i p_i,$$

$\alpha = \sum_{i=1}^4 \alpha_i e_i \in H$ , and geometrically

$$T = \mathbb{T}(H \cap \{\alpha_i \geq 0\})$$

$F : V \rightarrow V$  affine mapping.

$F$  lifts to a linear mapping

$$M : (U, H) \rightarrow (U, H)$$

preserving the hyperplane  $H$

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$M$  is defined uniquely by the commuting diagram

$$\mathbb{T}(M(\bullet)) = F(\mathbb{T}(\bullet))$$

$$F(p_i) = \sum_{j=1}^4 \alpha_{ji} p_j \text{ in barycentric coordinates } \alpha_{ji}.$$

Then

$$\sum_{i=1}^4 \sum_{j=1}^4 \alpha_{ji} p_j \otimes e_i^* = \sum_{j=1}^4 p_j \otimes \left( \sum_{i=1}^4 \alpha_{ji} e_i^* \right) = \sum_{j=1}^4 p_j \otimes M^*(e_j^*).$$

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### **Generation of tetrahedral chain**

$$s_i \text{ center of } S_i, s_i = \frac{1}{3}(\sum_{j=1}^4 p_j - p_i)$$

Four orthogonal reflections by  $S_i$

$$R_i(p) = p - 2 \frac{(p - s_i | s_i - p_i)}{(s_i - p_i | s_i - p_i)} (s_i - p_i)$$

$$R_i(p_j) = p_j + 2\delta_{ij} \left( \frac{1}{3} \sum_{k \neq i} p_k - p_j \right), \quad j = 1, \dots, 4$$

$\{T^{(i)}\}_{i=0}^n$  tetrahedral chain

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$$\begin{aligned}
T^{(0)} &= T, \\
T_{i_1}^{(1)} &= \bar{R}_{i_1} T, \\
T_{i_1 i_2}^{(2)} &= \bar{R}_{i_2} \bar{R}_{i_1} T, \quad i_1 \neq i_2, \\
&\dots \quad \dots \quad \dots \\
T_{i_1 i_2 \dots i_n}^{(n)} &= \bar{R}_{i_n} \dots \bar{R}_{i_2} \bar{R}_{i_1} T, \quad i_{k+1} \neq i_k, k = 1, \dots, n-1.
\end{aligned}$$

$\bar{R}_i : \mathcal{T} \rightarrow \mathcal{T}$  twist morphisms, defined by  $R_i$ .

### Representation in barycentric coordinates

$$\bar{R}_i : \mathcal{T} \rightarrow \mathcal{T}, \quad \bar{R}_i(v \otimes u^*) = v \otimes M_i^* u^*$$

$$M_1 = \begin{pmatrix} -1 & \frac{2}{3} & \frac{2}{3} & \frac{2}{3} \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}^T, \quad M_2 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ \frac{2}{3} & -1 & \frac{2}{3} & \frac{2}{3} \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}^T,$$

$$M_3 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ \frac{2}{3} & \frac{2}{3} & -1 & \frac{2}{3} \\ 0 & 0 & 0 & 1 \end{pmatrix}^T, \quad M_4 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \frac{2}{3} & \frac{2}{3} & \frac{2}{3} & -1 \end{pmatrix}^T.$$

$\bar{R}_i$  is represented by transpose of  $M_i$

### EXAMPLE

$$\bar{R}_1 \left( \sum_{i=1}^4 p_i \otimes e_i^* \right) = \sum_{i=1}^4 p_i^{(1)_1} \otimes e_i^*,$$

where

$$\begin{pmatrix} p_1^{(1)_1} \\ p_2^{(1)_1} \\ p_3^{(1)_1} \\ p_4^{(1)_1} \end{pmatrix} = \begin{pmatrix} -1 & \frac{2}{3} & \frac{2}{3} & \frac{2}{3} \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} p_1 \\ p_2 \\ p_3 \\ p_4 \end{pmatrix},$$

$$T_{i_1 \dots i_n}^{(n)} = \bar{R}_{i_n} \dots \bar{R}_{i_1} T.$$

### Coding in triplets of consecutive steps

$$T_k^{(r+1)} = \bar{R}_k T^{(r)}$$

$$T_{kj}^{(r+2)} = \bar{R}_j \bar{R}_k T^{(r)}$$

$$T_{kji}^{(r+3)} = \bar{R}_i \bar{R}_j \bar{R}_k T^{(r)}.$$

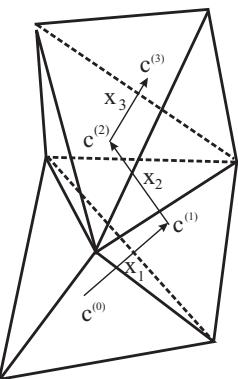
$$U, D, F : \quad T_{kji}^{(r+3)} = \bar{R}_i \bar{R}_j \bar{R}_k T^{(r)}$$

$$F : \quad T^{(r+3)}; \quad \det(x_{r+1}, x_{r+2}, x_{r+3}) = 0$$

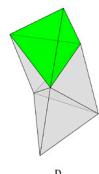
$$U : \quad T^{(r+3)}; \quad \det(x_{r+1}, x_{r+2}, x_{r+3}) > 0$$

$$D : \quad T^{(r+3)}; \quad \det(x_{r+1}, x_{r+2}, x_{r+3}) < 0$$

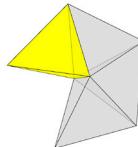
### Shape orientation



### Basic units



D



F



U

**Tetrahedral chains:** DDUF...UDFFD.

Combinatorial codes for U, D, F

Admissible triplets parametrizing U D F:

$$(k, i, j), 1 \leq i, j, k \leq 4, \quad k \neq j \neq i$$

## EXAMPLE

UUFD

$$(3, 4, 2) \rightarrow (4, 2, 1) \rightarrow (2, 1, 4) \rightarrow (1, 4, 1) \rightarrow (4, 1, 3).$$

$$T_{3421413}^{(7)} = R_3 R_1 R_4 R_1 R_2 R_4 R_3 T$$

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### Classification of admissible triplets

$u$	$d$	$f$
$\det(x_1, x_2, x_3) = 32\sqrt{3}/243$	$\det(x_1, x_2, x_3) = -32\sqrt{3}/243$	$\det(x_1, x_2, x_3) = 0$
$(k, j, i)$	$(k, j, i)$	$(k, j, i)$
$(3, 2, 1)$	$(4, 2, 1)$	$(1, 2, 1)$
$(4, 3, 1)$	$(2, 3, 1)$	$(1, 3, 1)$
$(2, 4, 1)$	$(3, 4, 1)$	$(1, 4, 1)$
$(4, 1, 2)$	$(3, 1, 2)$	$(2, 1, 2)$
$(1, 3, 2)$	$(4, 3, 2)$	$(2, 3, 2)$
$(3, 4, 2)$	$(1, 4, 2)$	$(2, 4, 2)$
$(2, 1, 3)$	$(4, 1, 3)$	$(3, 1, 3)$
$(4, 2, 3)$	$(1, 2, 3)$	$(3, 2, 3)$
$(1, 4, 3)$	$(2, 4, 3)$	$(3, 4, 3)$
$(3, 1, 4)$	$(2, 1, 4)$	$(4, 1, 4)$
$(1, 2, 4)$	$(3, 2, 4)$	$(4, 2, 4)$
$(2, 3, 4)$	$(1, 3, 4)$	$(4, 3, 4)$

### $U$ -chains period

$(3, 2, 1) \rightarrow (2, 1, 4) \rightarrow (1, 4, 3) \rightarrow (4, 3, 2)$
$(4, 3, 1) \rightarrow (3, 1, 2) \rightarrow (1, 2, 4) \rightarrow (2, 4, 3)$
$(2, 4, 1) \rightarrow (4, 1, 3) \rightarrow (1, 3, 2) \rightarrow (3, 2, 4)$
$(3, 4, 2) \rightarrow (4, 2, 1) \rightarrow (2, 1, 3) \rightarrow (1, 3, 4)$
$(4, 1, 2) \rightarrow (1, 2, 3) \rightarrow (2, 3, 4) \rightarrow (3, 4, 1)$
$(4, 2, 3) \rightarrow (2, 3, 1) \rightarrow (3, 1, 4) \rightarrow (1, 4, 2)$
$(1, 4, 3) \rightarrow (4, 3, 2) \rightarrow (3, 2, 1) \rightarrow (2, 1, 4)$
$(1, 2, 4) \rightarrow (2, 4, 3) \rightarrow (4, 3, 1) \rightarrow (3, 1, 2)$
$(1, 3, 2) \rightarrow (3, 2, 4) \rightarrow (2, 4, 1) \rightarrow (4, 1, 3)$
$(2, 1, 3) \rightarrow (1, 3, 4) \rightarrow (3, 4, 2) \rightarrow (4, 2, 1)$
$(2, 3, 4) \rightarrow (3, 4, 1) \rightarrow (4, 1, 2) \rightarrow (1, 2, 3)$
$(3, 1, 4) \rightarrow (1, 4, 2) \rightarrow (4, 2, 3) \rightarrow (2, 3, 1)$

### $D$ -chains period

$(2, 1, 4) \rightarrow (1, 4, 3) \rightarrow (4, 3, 2) \rightarrow (3, 2, 1)$
$(3, 1, 2) \rightarrow (1, 2, 4) \rightarrow (2, 4, 3) \rightarrow (4, 3, 1)$
$(4, 1, 3) \rightarrow (1, 3, 2) \rightarrow (3, 2, 4) \rightarrow (2, 4, 1)$
$(4, 2, 1) \rightarrow (2, 1, 3) \rightarrow (1, 3, 4) \rightarrow (3, 4, 2)$
$(1, 2, 3) \rightarrow (2, 3, 4) \rightarrow (3, 4, 1) \rightarrow (4, 1, 2)$
$(2, 3, 1) \rightarrow (3, 1, 4) \rightarrow (1, 4, 2) \rightarrow (4, 2, 3)$
$(4, 3, 2) \rightarrow (3, 2, 1) \rightarrow (2, 1, 4) \rightarrow (1, 4, 3)$
$(2, 4, 3) \rightarrow (4, 3, 1) \rightarrow (3, 1, 2) \rightarrow (1, 2, 4)$
$(3, 2, 4) \rightarrow (2, 4, 1) \rightarrow (4, 1, 3) \rightarrow (1, 3, 2)$
$(1, 3, 4) \rightarrow (3, 4, 2) \rightarrow (4, 2, 1) \rightarrow (2, 1, 3)$
$(3, 4, 1) \rightarrow (4, 1, 2) \rightarrow (1, 2, 3) \rightarrow (2, 3, 4)$
$(1, 4, 2) \rightarrow (4, 2, 3) \rightarrow (2, 3, 1) \rightarrow (3, 1, 4)$

## Combinatorial structure

$$\mathbb{I} = \{(\alpha, \beta) \in \Delta \times \Delta : \alpha \neq \beta\}$$

$$\Delta = \{1, 2, 3, 4\}$$

Uniquely defined mappings

$$L_u, L_d, L_f : \mathbb{I} \rightarrow \Delta, \quad \#\mathbb{I} = 12$$

and bijections

$$\mathcal{L}_u, \mathcal{L}_d, \mathcal{L}_f : \mathbb{I} \rightarrow \mathbb{I},$$

$$\mathcal{L}_*(i_1, i_2) = (i_2, L_*(i_1, i_2)), * = u, d, f.$$

## $\mathcal{L}$ - sequence for tetrahedral chain

Example

$$DUUFD \longrightarrow \mathcal{L}_d \mathcal{L}_f \mathcal{L}_u \mathcal{L}_d \mathcal{L}_d$$

**Any periodic tetrahedral chain is characterized by  
cycling composition of a numerical representation of  
its period**

Compositions of  $\mathcal{L}_*$ -sequences form the indexing space for tetrahedral chains

The indexing space is a binary tetrahedral subgroup of  $S_{12}$

generated by three elements  $\mathcal{L}_u, \mathcal{L}_d, \mathcal{L}_f$  with the relations

$$\mathcal{L}_u^3 = id, \quad \mathcal{L}_d^3 = id, \quad \mathcal{L}_f^2 = id, \quad (\mathcal{L}_u \mathcal{L}_d)^2 = id.$$

### Geometric characteristics

-proper tetrahedral chains

$n$	3	4	5	6	7	8	9	10	11	12	13
$A_n$	1	3	9	26	76	218	628	1802	5146	14670	41734

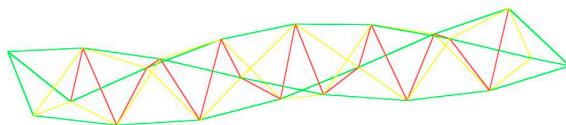
-branching order  $0 \leq b \leq 3$

-vertex order  $P(p)$ ,  $\sum_{p \in V_{C_n}} P(p) = 4n$

-clustering function

$$Cl(C_n) = \sum_{p \in V_{C_n}} \max(0, P(p) - 4)$$

## Tetrahelix

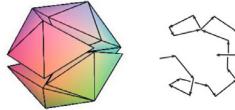


Zero branching order



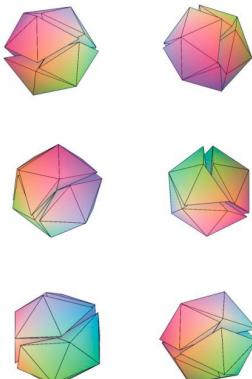
### Proper chains sharing one common vertex

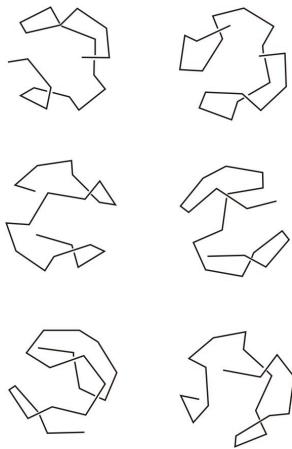
$b \setminus n$	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
1	0	0	0	0	0	1	2	6	9	19	38	49	69	79	71	34	6
2	0	0	1	4	6	10	24	46	78	113	137	153	132	85	36	6	0
3	2	4	6	9	16	27	38	48	55	56	50	35	22	12	2	0	0
total	2	4	7	13	22	38	64	100	142	188	225	237	223	176	109	40	6



### Ico-clusters

*FFUFFFDUDUDUFFDU, FFUFFDUDUDUDFFU  
UFFDFFUDUDUFFDFFU, UFFDUDFFUFFDUDF  
UDFFUFFDUDFFUFFDU, UDFFUFFDUDUDFFU*

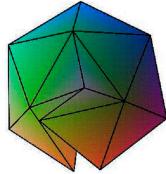




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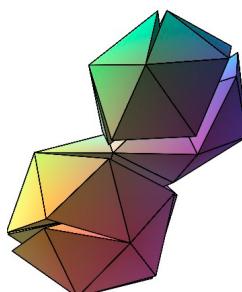
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Smallest unit  $b = 1$



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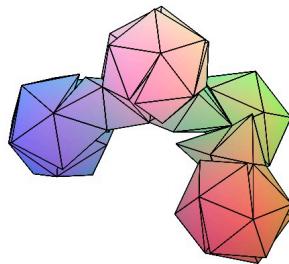
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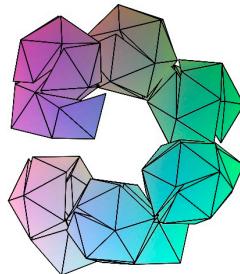
### Clustering folding



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### Clustering folding



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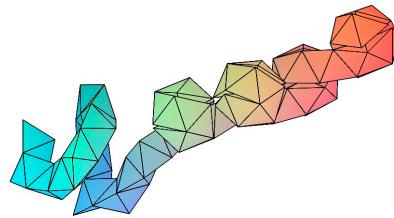
### Big periodic



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## Mixed clustering folding

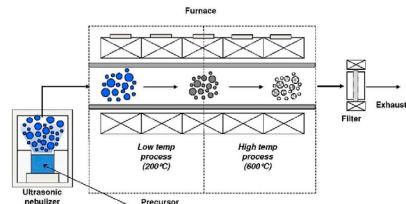


H. Babiker, S. Janeczko, **Combinatorial representation of tetrahedral chains**, *Communications in Information and Sciences*, Vol. 15, No. 3, (2015), 331-359

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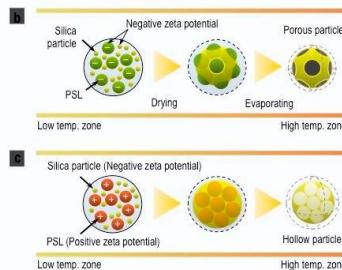
## Nano-blood particles



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## Spray technology



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## Silica particles

Sample	a	b	c	d	e	f
n	one	two	three	four	five	six
Silica particle						
Model						

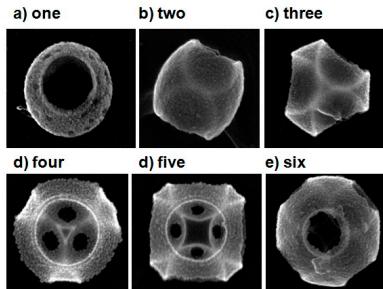
## Large silica particles

Sample	n = 4	n = 13	n > 14	n > 27	n > 35
Aggregated large silica particle					
a Model					

## Porous particles

Sample	n = 4	n = 13	n > 14	n > 27	n > 35
Aggregated large silica particle					
a Model					
b Porous particle					

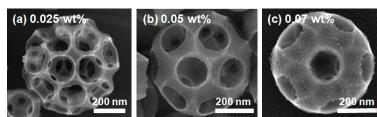
### Stable porous particles



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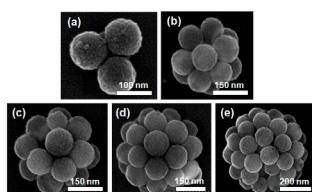
### Porous particles



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### Hollow particles



S.Y. Lee, L. Gradon, S. Janeczko, F. Iskandar, K. Okuyama, **Formation of Highly Ordered Nanostructures by drying Micrometer Colloidal Droplets**, *ACS Nano Journal*, Vol. 4, No. 8, (2010), 4717-4724

L. Gradon, S. Janeczko, M. Abdullah, F. Iskandar, K. Okuyama, **Self-Organization Kinetics of Mesoporous Nanostructured Particles**, *AIChE Journal* Vol. 50, No. 10, (2004), 2583-2593.

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Geometrical coding of DNA sequences

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Geometrical coding of DNA sequences

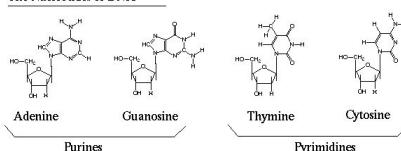
(1) UUUUUUUUUUUUUUUUUUUU(A, G) ACTACATACATACATAC  
 (1) UUUUUUUUUUUUUUUUUUUU(A, T) ATGACATAGATCTATGTAT  
 (1) UUUUUUUUUUUUUUUUUUUU(C, A) CAGCCGGCAGCACGCCA  
 (1) UUUUUUUUUUUUUUUUUUUU(C, T) CTACATACATCTCCATAC  
 (1) UUUUUUUUUUUUUUUUUUUU(C, G) GATGTCATGATGATGAT  
 (1) UUUUUUUUUUUUUUUUUUUU(T, A) TACTCATACATACATAC  
 (1) UUUUUUUUUUUUUUUUUUUU(T, C) GATGATGATGATGATGAT  
 (1) UUUUUUUUUUUUUUUUUUUU(T, G) TGACATGATGATGATGAT  
 (1) UUUUUUUUUUUUUUUUUUUU(G, A) GATGATGATGATGATGAT  
 (1) UUUUUUUUUUUUUUUUUUUU(G, T) GTCTGGCTCCGCTTCGCG  
  
 (1) UUUUUUUUUUUUUUUUUUUU(A, C) ACTCTACATACATACATAC  
 (1) UUUUUUUUUUUUUUUUUUUU(A, T) ATGATCTGCTGATGCTGAT  
 (1) UUUUUUUUUUUUUUUUUUUU(C, A) CAGACGAGCCGGCAG  
 (1) UUUUUUUUUUUUUUUUUUUU(C, T) CTACATACATCTACACTAC  
 (1) UUUUUUUUUUUUUUUUUUUU(C, G) GATGTCATGATGATGAT  
 (1) UUUUUUUUUUUUUUUUUUUU(T, A) TACTACATCTACATCTAC  
 (1) UUUUUUUUUUUUUUUUUUUU(T, C) GATGATGATGATGATGAT  
 (1) UUUUUUUUUUUUUUUUUUUU(T, G) TGACATGATGATGATGAT  
 (1) UUUUUUUUUUUUUUUUUUUU(G, A) GATGATGATGATGATGAT  
 (1) UUUUUUUUUUUUUUUUUUUU(G, T) GTCTGGCTCCGCTTCGCG  
  
 (1) UUUUUUUUUUUUUUUUUUUU(A, C) ACTCTACATACATACATAC  
 (1) UUUUUUUUUUUUUUUUUUUU(A, T) ATGATCTGCTGATGCTGAT  
 (1) UUUUUUUUUUUUUUUUUUUU(C, A) CAGACGAGCCGGCAG  
 (1) UUUUUUUUUUUUUUUUUUUU(C, T) CTACATACATCTACACTAC  
 (1) UUUUUUUUUUUUUUUUUUUU(C, G) GATGTCATGATGATGAT  
 (1) UUUUUUUUUUUUUUUUUUUU(T, A) TACTACATCTACATCTAC  
 (1) UUUUUUUUUUUUUUUUUUUU(T, C) GATGATGATGATGATGAT  
 (1) UUUUUUUUUUUUUUUUUUUU(T, G) TGACATGATGATGATGAT  
 (1) UUUUUUUUUUUUUUUUUUUU(G, A) GATGATGATGATGATGAT  
 (1) UUUUUUUUUUUUUUUUUUUU(G, T) GTCTGGCTCCGCTTCGCG

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The Nucleotides of DNA



A ≡ Adenine, T ≡ Thymine, C ≡ Cytosine, G ≡ Guanine

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