## Nanostructured surfaces

# Packing and percolation of interacting linear k-mers on a square lattice

**N.V. Vygornitskii[1], S. Khrapatiy[2], N. Lebovka[1]**

[1]*Institute of Biocolloidal Chemistry named after F. D. Ovcharenko, Natl. Acad. of Sci. of Ukraine. 42, Vernadsky av., 03142, Kyiv, Ukraine*
*E-mail: vygornv@gmail.com*
[2]*Taras Shevchenko National University of Kyiv, Institute of Biology, 2, prospekt Hlushkov, Kyiv, 03022, Ukraine*

Packing and percolation problems for deposited *k*-mers (elongated particles occupying *k* adjacent sites), continuously attract great interests [1-3]. Particular interest was recently originated to the investigation of model accounting for the repulsive or attractive interactions between different *k*-mers. Theses models offer an attractive perspective for description of nanostructured surfaces including nanotubes, charged nanodisks (e.g., laponite) or proteins. The reported work utilised random sequential adsorption (RSA) model for deposition of *k*-mers in the sites of a square lattice. In RSA model the species are placed randomly such that they do not overlap with any of previously deposited. The nearest-neighbour attractive and repulsive interactions between different *k*-mers were taken into account. These interactions were characterized by the parameters $\varepsilon_a$ (attractive) and $\varepsilon_r$ (repulsive). The minimum concentration $p_c$ for which a spanning cluster formed (percolation concentration) and maximum available packing fraction $p_j$ (jamming concentration) were determined. The percolation threshold $p_c$ was calculated by using the Hoshen and Kopelman algorithm; the thermodynamic limits for $p_c$ and $p_j$ were evaluated using the standard finite scaling procedures. The dependencies of the packing and percolation concentration and the average coordination numbers versus interaction parameters were investigated. In summary, the proposed model seems to be a promising for prediction of non-equilibrium states and percolation properties of the system for attractive and repulsive interactions.

The author acknowledges the partial financial support of project 43-02-14(U), Ukraine.

1. *Lebovka, N., Karmazina, N., Tarasevich, Yu., Laptev, Yu.* Random sequential adsorption of partially oriented linear k-mers on a square lattice // Phys. Rev. E -2011. -**84**. -P 29902.

2. *Tarasevich, Y., Lebovka, N., Laptev, V.* Percolation of linear k-mers on a square lattice: From isotropic through partially ordered to completely aligned states, Phys. Rev. E – 2012. -**86**. –P. 61116.

*3. Lebovka, N., Khrapatiy, S., Vygornitskyi, N. Pivovarova, N.,* Barrier properties of k-mer packings // Physica A -2014. -**408.** -19-27.