**NUMER IDENTYFIKACYJNY // CONTRIBUTION ID**

**The new nanorocket propulsion mechanism based on fast water expulsion from hydrophobic porous materials**

Yuriy G. Bushuev, Mirosław Chorążewski,Yaroslav Grosu

*Institute of Chemistry, University of Silesia in Katowice, Szkolna 9 street, 40-006 Katowice, Poland*

yuriy.bushuev@us.edu.pl

The design and manufacturing of nanoscale rockets and motors are a fast-developing branch of nanoscience with applications in biology, medicine, environmental science, defense, and industry.[1] A nano rocket is a vehicle that obtains thrust from a tubular engine. Several mechanisms were proposed to stimulate nanoparticle movement. These nanodevices can be utilized as drug-delivering vehicles for killing cancer cells or bacteria, chemical sensors, and many other applications.

We present results based on observing fast water expulsion from hydrophobic nanopores during MD simulations of heterogeneous hydrophobic systems (HHSs) that combine hydrophobic porous solids and water. These systems are used to store mechanical and thermal energy and convert one into the other. Water penetrates a hydrophobic porous material only at elevated pressure. Extrusion can occur with pressure releases.

   

Figure 1: Snapshots illustrate water expulsion from a nanopore and a capped carbon nanotube. The specially colored water molecules have a speed of 30-70 m/s. Two jets of water are expelled through the nanopore from both sides. Water propels the carbon nanotube.

The results of the computer simulations we have performed demonstrate that water in hydrophobic pores is in a metastable state and can be ejected from pores with high velocity.[2,3] The illustrations are presented in Fig. 1. Analysis of the structure of water in hydrophobic nanopores, the study of water clustering, the stability of clusters, and the establishment of the role of spontaneous dipole-dipole reorientations allowed us to assume that the maximum of the microwave absorption band of pure water (about 19 GHz) is significantly shifted towards lower frequencies in the case when water fills pores. Thus, it is possible to heat confined water predominantly. Meanwhile, net water is more transparent in this frequency band. Heated metastable water is expelled from the material, pushing micro/nano rockets. After a short microwave radiation impulse and temperature relaxation, water penetrates pores again, and the process can be repeated. The particle direction of movement coincides with the direction of microwaves because water heating occurs only in pores lying along the radiation beam. The proposed mechanism is expected to be exploited for micro and nanorockets due to the scalability of porous materials, which can be zeolite crystals, grafted silica nanoporous particles, or bunches of nanotubes. The observed phenomena can be used for local water heating in porous membranes to enhance their permeability and productivity.

**Acknowledgements**.  This work has received funding from the European Union’s Horizon 2020 research and innovation program under grant agreement no. 101017858. We gratefully acknowledge the Polish high-performance computing infrastructure PLGrid (HPC Centers: WCSS, ACK Cyfronet AGH) for providing computer facilities and support within the computational grant no. PLG/2024/017096.

**References**

[1] J. Li, I. Rozen, I., J. Wang. “Rocket science at the nanoscale. In: *ACS Nano,* 2016, 10, p. 5619. doi: <http://dx.doi.org/10.1021/acsnano.6b02518.>

[2] Y. G. Bushuev, Y. Grosu, M. Chorążewski. “Spontaneous dipole reorientation in confined Water and its effect on wetting/dewetting of hydrophobic nanopores”. In: *ACS Appl. Mater. Interfaces,* 2024, 16, p. 7604.

doi: <http://dx.doi.org/10.1021/acsami.3c17272.>

[3] A.R. Lowe, M. Chorążewski, Y. Grosu, Y. G. Bushuev. “Energetic characteristics of hydrophobic porous materials as candidates for manufacturing of nanorockets ̇”. In: *J. Phys. Chem. Lett.* **2024**, *15*, p. 12112.

doi: <http://dx.doi.org/10.1021/acs.jpclett.4c02581.>