MOLECULAR SIMULATION STUDY OF LDH INTERCALATED WITH PORPHYRINS

MIROSLAV POSPÍŠIL[1]*, PETR KOVÁR[2]

[1]*Charles University in Prague, Prague, 12116, Czech Republic*
[2]*Charles University in Prague, Prague, 12116, Czech*
republic pospisil@karlov.mff.cuni.cz

Molecular calculations were used for structure analysis of various intercalated layered structures of layer double hydroxides (LDH) with different porphyrin anions. Simulations bring a detailed insight into the structure arrangement of the interlayer space and on the surface. We can analyze mutual interactions between inorganic layers and organic species, their charge distribution, energy characteristics, distribution function, influence of water on the stability of structure. Simulations were done in Cerius2 and Materials Studio modelling environment. Resultant calculated structures were carefully derived on the base of experimental results and presented models are in a good agreement with them. Knowledge of structure - properties relationship is crucial for explanation of physical properties of inorganic-organic hybrid materials [1].
Quantum mechanics and molecular modeling calculations combined with X-ray diffraction, thermogravimetry and electron density measurements were used for structure analysis of (i) Mg-Al LDH intercalated with [5,10,15,20-tetrakis(4-sulfonatophenyl)porphyrin (TPPS)], (ii) Zn2-Al LDH intercalated with porphyrin anions [Zn(II)-5,10,15,20-tetrakis(4-sulfonatophenyl) porphyrin – (ZnTPPS)] and (iii) both types of LDH intercalated with Pd-TPPS and Pd-TPPC (carboxyphenyl). The high crystallinity achieved upon hydrothermal treatment allowed us to give further insights into the interlayer structural arrangement of porphyrin guests. Porphyrins intercalated into LDH are producers of singlet oxygen with sufficient long lifetime. So, these hybrid materials create antibacterial environment [1] and are usable in medicine applications.

[1] Kovár P., Pospíšil, M., Káfuková, E., Lang, K., Kovanda F., Journal of Molecular Modeling, 2010, 16, 223-233.

Keywords: porphyrin, LDH, molecular simulations