

## Molecular simulations of layered materials intercalated with organic species

MILAN PŠENIČKA<sup>1\*</sup>, MIROSLAV POSPÍŠIL<sup>1</sup>,  
KLÁRA MELÁNOVÁ<sup>2,3</sup>

<sup>1</sup> Charles University in Prague, Faculty of Mathematics and Physics, Ke Karlovu 3, 121 16 Prague 2, CZ,

(\* correspondence: milan.psenicka@matfyz.cz)

<sup>2</sup> Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Heyrovsky Sq. 2, 162 06 Prague 6, CZ

<sup>3</sup> Present address: Joint Laboratory of Solid State Chemistry, Studentská 95, 53210 Pardubice, CZ

In our recent works we use molecular simulation methods to describe layered materials intercalated with organic species, especially those materials where the level of disorder prevents their description by direct experimental methods. Here, we will present Zn<sub>2</sub>Al/Mg<sub>2</sub>Al - Layered Double Hydroxides (LDH) intercalated with Pravastatin anions and Sr-phenylphosphonate intercalated with 1,2-alkanediols.

LDHs are very interesting matrices which to be explored as drug nanocarriers due to their biocompatibility and stability. The anionic forms of bioactive drugs can be intercalated into interlayer to store them and preserve drug decomposition. Intercalation of pravastatin drug into LDH was performed in [1] by co-precipitation method.

Metal phosphonates represent group of compounds playing an important role in the design of two-dimensional inorganic-organic hybrid materials. The applicability of the layered phosphonates can be increased by intercalation of commercially interesting, for instance optically or pharmaceutically active molecules. We present influence of intercalated 1,2 alkanediol on changes in structural arrangement of Sr phenylphosphonate.

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[1] CUNHA *et al.* (2012), *Chem. Mater.*, vol. 24, 1415–1425.