

## Abstract

**Title:** *Application of Molecular Simulations in Complex Structural Analysis of Layered Materials*

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**Abstract:**

Techniques of molecular simulations were used together with experimental measurements (X-ray diffraction, thermogravimetry, infrared spectroscopy, elemental analysis and others) to clarify the structure properties of various types of layered materials.

The structure of Zn-Al-layered double hydroxide intercalated by pyrenetetrakisulfonate acid was solved. Depending on the relative humidity, the samples showed different arrangements with three planes of water molecules and with either one or two planes of pyrenetetrakisulfonate anions. At the same time considerable variability of anions arrangement was demonstrated.

The adsorption behavior of natural montmorillonite and montmorillonite modified by tetramethylammonium cations in relation to aniline and phenol was explored. Adsorption features differed according to both the type of adsorbed molecules and the type of adsorbents. An important role was played by the plane of water molecules right above the surface which mediated adsorption of anilines. The water plane area was reduced by presence of tetramethylammonium cations which caused reduction of aniline adsorption. By contrast, the cations presence slightly increased adsorption of phenols.

The structure of strontium phenylphosphonate intercalated by diols with different length and with hydroxyl groups on the terminal carbon atoms was solved. Regarding ethanediols and propanediols, there was a strong interaction of one of their hydroxyl groups with two strontium atoms in the layer; the second hydroxyl group of ethanediol interacted with one strontium atom, while in propanediols the hydroxyl group formed hydrogen bonds with water molecules above the layer. For longer diols, both hydroxyl groups formed these hydrogen bonds; in butanediols towards only one layer, while in diols with more than six carbon atoms towards opposing layers, with the diols stretched diagonally across the interlayer.

**Keywords:** structure analysis, molecular simulations, intercalation, layered double hydroxide, pyrenetetrakisulfonate acid, montmorillonite, strontium phenylphosphonate