ENERGY THEORY OF SCROLLING: A TOOL FOR LAYERED COMPOUND MORPHOLOGY FORECAST

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Recently, increased attention has been paid to the scrolling of crystalline layers of varying chemical compositions, which occurs due to internal or external factors, as well as a combination of both. Unlike the more widely known nanotubes, the scrolled nature of the layer allows for extensive morphological modification: scrolling at various angles, scrolling with a variable radius of curvature, and response to changing external conditions. Partial loss of translational symmetry by the layer are also of fundamental interest in connection with the applicability, in this case, of the classical definition of the thermodynamic phase of matter.

Despite the wide diversity of compositions and structures, the class of nanoscrolls is currently presented in the literature more as a collection of disparate studies than as a unified whole. In this regard, the first part of the report formulates the fundamental equations of the energy theory of scrolling and attempts to apply them (at a qualitative level) to various currently known cases of scrolls formation from graphene, C_3N_4, MXenes, chalcogenides, oxides, layered double hydroxides, and other compounds. The second part focuses on the objects fundamental to this theory – phyllosilicates [1,2]. The following cases are considered:

– Correlation of the energy effect of scrolling and Calvet calorimetry data for $Mg_3Si_2O_5(OH)_4$ with the chrysotile structure;
– Isovalent and heterovalent substitution in the structure of phyllosilicates as a method for controlling morphology;
– Comparison of the energetic and thermodynamic factors of the formation of the distribution of substituting cations over a layer of variable curvature;
– Prediction of the scrolling potential and dimensional characteristics of nanoscrolls of 2:1 layered silicates (with talc and montmorillonite structures).

1. Krasilin A.A., Khrapova E.K., Maslennikova T.P. Cation Doping Approach for Nanotubular Hydrosilicates Curvature Control and Related Applications // Crystals. 2020. Vol. 10, Nr 8. P. 654. https://doi.org/10.3390/cryst10080654

2. Bloise A., Fuoco I., Apollaro C., Vespasiano G., Khrapova E., Krasilin A. Retrospective of chrysotile synthesis: From tough geoinspired process up to soft chemical design // Applied Clay Science. 2026. Vol. 281. P. 108088. https://doi.org/10.1016/j.clay.2025.108088