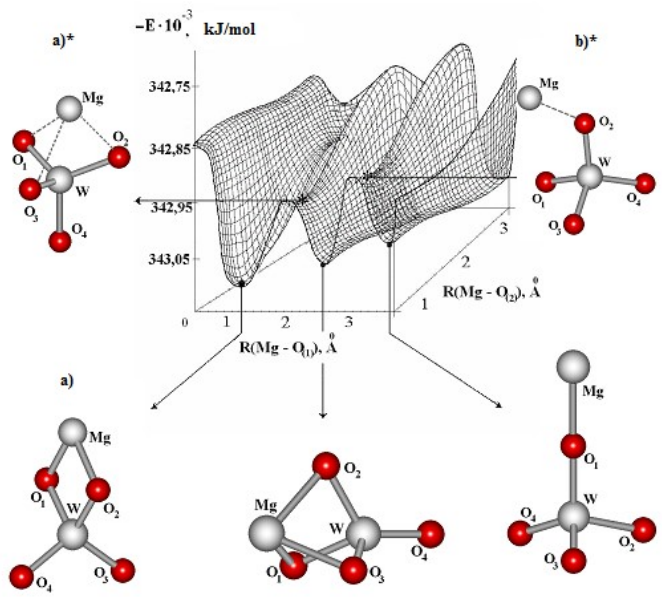
Physico-Chemical nanomaterials science

The life time of electrochemically active complexes, with multi-electron charge transfer in the process of obtaining new nanomaterials at HES

Earlier [1,2] it was substantiated the possibility of obtaining new nanomaterials by high-temperature electrochemical synthesis (HES). The decisive role in this case belongs to the cationic composition of the melt, an alternative to 6-electron charge transfer (simultaneous and sequential), which was determined by the lifetime of electrons $\Delta\tau$ in intermediate states. In this work, the results of the influence of the lifetime of electrons in intermediate states on the processes of multi-electron sequential charge transfer at HES for obtaining new polymorphic nanomaterials are presented.



An example of a part of the surface of the potential energy of the interaction Mg^{2+} ... WO_4^{2-} (Configuration a) corresponds to the absolute minimum, b) and c) to the local minima of the PES of the Mg^{2+}... WO_4^{2} interaction; a) * and b) * - system transition states)

Conclusion: Energy assessment of the advantage of simultaneous 6-electron charge transfer, in comparison with stepwise transfer, which takes into account the lifetime of intermediate intermediates, allows to obtain more complete information when obtaining new nanomaterials.

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2. Soloviev V.V., Solyanik L.A., Kuznetsova, T. Yu.,Holik, Yu.S., Illyash O.E., Usenko D.V. The effect of multielectron transfer on the direction for the mechanism of heterogeneous reactions during the synthesis for nanomaterials from tungstate melts under the conditions of cationic catalysis, - Molecular Crystals and Liquid CrystalsVolume 673, Issue 1, Pages 61 – 69, 22 September 2018.

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