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Advantages of Using Semi-Empirical Methods in Teaching Students at the Faculty of Chemistry of Uzhhorod National University

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Abstract

Background:

Semi-empirical methods of research of the properties of substances are applied during the occupations in scientific circles and play an important role in the training of students of the Faculty of Chemistry of Uzhhorod National University and also at implementation of academic year and degree projects.

The aim of the study – establishment of advantages of semi-empirical methods of a research of physicochemical properties of inorganic compounds over classical and alternative modern approaches.

Methods:

In the course of this work the calculation methods were used which are stated in the monographs by Viktorov (Methods of Calculation of Physicochemical Values and Applied calculations, 1977), Morachevskiy and Sladkov (Thermodynamic Calculations in Metallurgy, 1985), Zuyev, Potseluyeva, and Goncharov (The Crystal Energy as a Basis for Assessing the Properties of Solid Materials (including Magnesium Cements), 2006).

Results:

By results of processing of the known data and the carried-out comparative analysis it is established that semi-empirical methods of a research of physicochemical properties of substances have a number of advantages over available experimental and alternative calculation methods. The main of them are given below.

1. High expressivity. Implementation of calculations by means of semi-empirical methods needs insignificant time expenses. For example, modern non-empirical (ab initio) methods is more long-playing and bulky in essence. Experimental methods also longer in time also demand considerable expenses of material resources.
2. Rather high precision. Semi-empirical methods are characterized by rather low error within 5–10%. Possibly, ab initio methods have approximately the same or a little lower accuracy. Devices are available to pilot studies mainly belong to the Soviet period and do not meet modern requirements any more. Their error can fluctuate within 10–20 % or even to be higher.
3. The possibility of subsequent optimization and adaptation to new objects. Accuracy of the general semi-empirical methods can be increased, as a result of their adaptation to narrower circle investigated objects.
4. Simplicity of performance. Use of semi-empirical methods demands existence of a small amount of output experimental data. The most difficult

calculations come down to a conclusion of basic coefficients in the corresponding equations. Non-empirical methods need in more difficult actions and demand much stronger computers. Experimental methods are connected with synthesis, identification and next research of a certain physicochemical parameter. It demands new modern devices, each of which is ten times more expensive the personal computer sufficient than functionality.

5. Economy of expendables. By means of semi-empirical methods it is possible to minimize significantly the volume of pilot studies or, in certain cases, to do without them. It allows saving reactants, to reduce depreciation of devices and to focus attention only on the most perspective samples.

Conclusions:

Five main advantages of semi-empirical methods of a research of physicochemical properties of substances over classical and alternative modern approaches are established. It allows recommending the specified methods for active use in educational and research activity.

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