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Topological approach for the design of new materials

Vladislav A. Blatov[1]
[1]*Samara University, Samara, Russian Federation*
E-mail: blatov@gmail.com

Modern materials science provides new challenges to researchers in rational design of new compounds, structures and materials. It requires new methods of data processing to make the design as much reliable and predictive as possible. These methods should be implemented in new electronic tools – special software and databases. Importantly, an essential progress can be made in this field with crystallographic data.

At present, a huge amount of experimental information on crystal structures is collected in world-wide crystallographic databases, a total of more than one million entries. These are the primary data obtained directly in a diffraction experiment in the form of space group, unit cell parameters, atomic coordinates, etc. They are being extended with the data on physical properties of crystalline substances, but these data are also just a result of measurement. At the same time, the primary information contains a lot of hidden regularities, and indeed we need new tools to reveal them. With these tools we will be able to transform the crystallographic databases into knowledge databases containing correlations and rules, which then could be used for prediction of new substances and materials.

In crystal chemistry, such correlations usually follow the general form 'chemical composition – structure – physical property', where the middle term is crucial. Indeed, if chemical composition and physical property can be easily and strictly defined, the terms 'crystal structure' or 'local atomic structure' require a large number of descriptors. Thus we need to invent as many robust descriptors derived from structural data as possible. Here we consider one of the most important groups of such descriptors, the topological ones. They can be derived from the primary crystallographic data and supply them with the information on the structure connectivity, which is one of the main and natural chemical and crystallochemical characteristics. Another important feature of topological descriptors is that they allow one to formalize the classification of crystal structures and search for structural correlations.

We explore how the topological information is derived from the crystallographic data, stored in topological databases and then used for prediction of crystal structures. We discuss hybrid topological-DFT methods, which include fast screening of topological databases and subsequent precise estimation of physical properties by DFT modeling. Examples from different classes of chemical compounds are presented: ionic substances, intermetallics, ion conductors, microporous materials, coordination polymers, molecular crystals. A route to uniting crystallographic and topological knowledge within the same universal storage is outlined.

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