DATA-MINING APPROACHES TO FIND NEW FUNCTIONAL MATERIALS

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Progress in materials science is with few exceptions primarily driven by experimental exploration that is followed by theoretical work. Unfortunately, theory seldom leads the way forward in identifying or predicting materials with desired functionality, albeit a few exceptions to this rule exists. For instance, the observed tunneling magneto resistance in Fe/MgO/Fe sandwich structures, where a few layers of insulating MgO is inserted between thin films of Fe, was an experimental realization that followed theoretical predictions, based on calculations of the electronic structure. Graphene, the celebrated two-dimensional material, where many of the observed exotic properties are the result of a linear dispersion of the electron states around the Fermi level, is another example where theory of the exotic electronic structure preceded experimental measurements.

Unfortunately, the list of examples where theory actually makes predictions of new materials or new properties, is very short. New tools and new ways to work are clearly needed to improve the rate with which new materials may be identified, and theory may play a crucial role. A method that quickly is being established, involve data-mining algorithms and advanced, high-throughput electronic structure theory. The fundamental ideas behind this method [2] are described in this talk, and examples will be given of how it has so far been found to perform.

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1. RCTP-15 web site, `http://www.ihed.ras.ru/rctp2018/en/contribution`
2. O.Eriksson, Nature Nanotechnology **13**, 180 (2018)