New data mining resource for organic materials available

March 6 2017

A new, freely accessible database of organic and organometallic materials' electronic structures is now available online for research with quantum materials.

Published by the Condensed Matter research group at the Nordic Institute for Theoretical Physics (NORDITA) at KTH Royal Institute of Technology in Sweden, the Organic Materials Database is intended as a data mining resource for research into the electric and magnetic properties of crystals, which are primarily defined by their electronic band structure—an energy spectrum of electrons motion which stem from their quantum-mechanical properties.

Computer calculation of such structures is difficult and demands large computational resources. But thanks to advances in computational power and a high demand for prediction of materials with target properties, a new way of dealing with quantum materials has developed. Materials informatics focuses on performing – and developing tools for – high-throughput computing and data mining.

"You can think of it as aggregate informatics analysis, where the properties of a single compound are captured approximately and resources are aimed toward understanding global trends within the large datasets," says Alexander Balatsky, Professor of Theoretical Physics at KTH.

Applications of this informatics-driven approach are wide-ranging and

cover, for example, the search for various functional materials with special electrical, optical and magnetic properties, including the 2016 Nobel Prize-winning topological states of matter – an important building block of a quantum computer.

The database will facilitate the first-principles investigation of organics and the prediction of organic functional materials, given their high potential for industrial applications, Balatsky says.

Electronic band structures are calculated using density functional theory that is a standard tool in modern materials science. The OMDB web interface allows users to search for materials with specified target properties using non-trivial queries about their electronic structure, including advanced tools for pattern recognition, chemical and physical properties search.

More information: Stanislav S. Borysov et al. Organic materials database: An open-access online database for data mining, *PLOS ONE* (2017). DOI: 10.1371/journal.pone.0171501

Data Mining for 3D Organic Dirac Materials: Focus on Space Group #19. arxiv.org/abs/1611.04316

Provided by KTH Royal Institute of Technology