The mathematical design of new materials

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Short Report

This six-month program brought together participants with diverse expertise, including applied mathematics, physics, chemistry and engineering, all interested in materials with unusual properties. The main focus of the programme has been on the design of new materials, rather than just understanding of existing ones. The program was composed of four main academic workshops, two Newton Gateway knowledge-exchange events and one Spring School, all sharing a common theme: design of materials.

During the first and second workshops and the first Newton Gateway event the primary subjects were: a) mathematical design of new phase transforming materials with emerging applications to medical devices, and b) phase-transforming multiferroic materials used in energy conversion devices. A mini-symposium within the satellite workshop at Edinburgh focused on machine learning approaches for algorithmic design of new materials. It showed that more and more experimentalists adapted to the rational material design strategy guided by the cofactor conditions (a set of mathematical conditions on material structural parameters).

Thanks to the first knowledge exchange event, industry participants established close connections to the academical participants. For example, Andrew Bissell, the CEO of Sunamp Ltd. on renewable thermal energy storage, showed great interest on the energy conversion by first-order phase transforming ferroelectrics. After the event, there were some further connections and he sent his engineers to the Edinburgh satellite workshop and spring school for absorbing new mathematical ideas with application to thermal batteries.

Soft matter was an important part of the research programme, especially focusing on topics of active and passive complex fluid materials. Research was performed along multiple research themes, such as mathematics of colloids in nematic fluids, topology and topological defect as signatures of material frustration, microfluidic application of complex fluids, active matter and active fluids, role of molecular and micro-material design and shape control by liquid crystal elastomers. As part of activities on soft matter, a workshop on Optimal design of soft matter - including a celebration of Women in Materials Science (WMS) was organised that featured invited and contributed talks from top-level international speakers.

Overall we discovered a multifaceted approach to design: in mathematics, the design is based on the minimization and optimization problems in the framework of calculus of variations; in engineering, the design is a process of trial-test-correction; in physics and mechanics, the design is related to understanding and proposing a constitutive law. Researchers from all over the world use their own tools to solve similar design problems, but here at Newton Institute they were joined together to study the “foreign” languages of different field to find the common ground and initiate new “chemistry” among them leading to fruitful collaborations and possible new breakthroughs in the field of material design.