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# Smart materials design in non-linear optics for telecommunications

**Jacqueline M. Cole**
University of Cambridge, UK

This paper illustrates a range of methods that are being employed in order to systematically discover new classes of organic and organometallic non-linear optical (NLO) materials, with a particular interest in frequency-doubling applications. The importance of engaging in the full 'life-cycle' of materials prediction, experimental validation and NLO performance rationalisation, in order to afford success in this materials discovery program, is illustrated by several case studies.

Large-scale data-mining methods which are able to predict new organic NLO materials are presented together with results from subsequent NLO performance testing. Such experimental validation is complemented with quantitative structure-property relationship (QSPR) methods that have a dual function:- to help to rationalise the experimental results and to provide new design rules that are then fed back into the materials prediction aspect of this work. The 'life-cycle' of the materials discovery process then repeats via this feedback-loop creating a continuous 'design-to-device' operational program.

An overview of the prediction methods includes a demonstration of how large-scale quantum-chemical calculations can reveal new classes of NLO materials. A new way of calculating NLO performance indicators from empirical equations which is fast enough for an alternative, more sophisticated large-scale data-mining strategy is also presented. This same method is also shown to be able to derive a solid-state measure of NLO effects via experimental X-ray diffraction data that is modelled via a charge-density analysis.

The paper concludes with an outlook on future developments in materials discovery in the context of this field of research.

## Biography

Jacqui Cole is Head of the Structure and Dynamics group at the Cavendish Laboratory. She is engaged in the design and functionalisation of new materials for optoelectronic applications, with particular interests in (a) non-linear optics, (b) dye-sensitised solar cells, (c) optical data storage. She uses a wide variety of experimental and computational techniques to realise this goal. Experimental techniques include X-ray and neutron diffraction, anomalous X-ray scattering, EXAFS, XANES, solid-state NMR, FTIR, inelastic neutron scattering. Computational techniques include data-mining, Monte Carlo simulations and density-functional theory modelling.

jmc61@hermes.cam.ac.uk