School of Chemistry and Biochemistry
University of Windsor
273-1 Essex Hall
401 Sunset Avenue
Windsor
Ontario
Canada
N93 3P4

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Dear Professor Keen,

I am writing to you to apply for the 2011 PANalytical Thesis Prize in Physical Crystallography. Please find enclosed an electronic copy of my thesis, on CD-ROM, and a copy of my personal statement, as requested. I would like to use my PhD supervisors Professor Philip Lightfoot and Dr Sharon E. Ashbrook as academic referees, their contact details are listed below. Please do not hesitate to contact me if you have any questions regarding my thesis. My email address is karenjohnston980@gmail.com.

Professor Philip Lightfoot
School of Chemistry
University of St Andrews
North Haugh
St Andrews
Fife
KY16 9ST
Email: pl@st-andrews.ac.uk
Phone: 01334 463841

Dr Sharon E. Ashbrook
School of Chemistry
University of St Andrews
North Haugh
St Andrews
Fife
KY16 9ST
Email: sema@st-andrews.ac.uk
Phone: 01334 463779

Yours sincerely

K Johnston

Karen Johnston

The thesis entitled 'A Complementary Study of Perovskites: Combining Diffraction, Solid-State NMR and First-Principles DFT Calculations' should be considered for the PANalytical Thesis Prize in Physical Crystallography because it demonstrates the importance of combining several different characterisation techniques and highlights the necessity of applying a multidisciplinary approach to research. The work presented in the thesis focuses on the synthesis and structural characterisation of different perovskite systems, including $NaNbO_3$, $LaScO_3$, and their related solid-solutions.

Physical crystallography was undoubtedly key to the success of the work presented within the thesis. The combined use of high-resolution X-ray and neutron powder diffraction, Rietveld analysis and structural refinement enabled accurate and detailed structural information to be obtained for each of the systems investigated. Neutron powder diffraction, in particular, proved to be vital throughout this investigation. Neutron diffraction is often used for the study of complex perovskite-based systems as it is widely known to enhance superstructure peaks and can, therefore, offer additional structural information typically lost when using conventional X-ray methods alone. For example, using neutron diffraction it was possible to distinguish between two very similar polymorphs of $NaNbO_3$. The successful identification of the two phases enabled the structure of each to be determined by structural refinement using Rietveld analysis. Physical crystallography therefore played a crucial role in the structural determination of each of the systems investigated.

The application of complementary techniques such as solid-state NMR throughout the structural study enabled the short-range order of each system to be probed. Conventional MAS and high-resolution two-dimensional ^{23}Na, ^{93}Nb, ^{45}Sc and ^{17}O MAS NMR experiments were completed for each of the systems investigated, each of which provided useful additional structural information not generally accessible when using conventional diffraction techniques alone. Using the two techniques in conjunction with one another enabled a more detailed and comprehensive structural investigation to be completed for each system.

Density functional theory (DFT) calculations are a convenient way of directly linking diffraction and NMR. The CASTEP code, for example, is a planewave DFT code that exploits the inherent periodicity of many solids and enables the accurate calculation of NMR parameters. First-principles DFT calculations were therefore used in conjunction with experimental methods. The NMR parameters calculated aided with both the assignment and interpretation of often complex experimental NMR spectra. DFT calculations were therefore hugely valuable throughout the investigation.

The successful completion of the thesis was undoubtedly due to the use of a combined approach. The use of multiple techniques enabled information that is typically lost when using solely one characterisation method to be gained. Using physical crystallography, in conjunction with other complementary techniques such as solid-state NMR and DFT calculations, each system was successfully and comprehensively characterised. Physical crystallography was therefore essential to the success of the work presented within the thesis.