Integrated Materials Design Centre Seminar

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VACANCIES JOB IN OXIDE PEROVSKITE THIN FILMS

Dr Claudio Cazorla

School of Materials Science and Engineering,
University of New South Wales

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Time: **1:00 pm - 2:00 pm**
Venue: **320, Chemical Sciences Building (F10)**

Point defects can affect considerably the structural, magnetic, and transport properties of perovskite-structure materials with chemical formula ABO3. Oxygen vacancies (VO), for example, enable ionic conductivity in perovskite-based solid solutions to be used for electrochemical applications such as solid oxide fuel and electrolysis cells [1]. Likewise, V_O can distort significantly the equilibrium arrangement of atoms and hence modify the superexchange interactions between neighboring magnetic ions [2]. Engineering of defects in perovskite oxides, therefore, emerges as a likely avenue for the design of new materials with tailored functionality.

Recently, it has been experimentally demonstrated that strain engineering can be used to tune the content of oxygen in some perovskite oxides. For example, in $SrCoO_{3-\delta}$ thin films, a moderate epitaxial strain of about +2% produces an approximate 30% reduction in the oxygen activation energy barrier, which makes it possible to stabilize oxygen-deficient samples at annealing temperatures close to ambient conditions [3]. Also, in multiferroic $SrMnO_3$ thin films the formation energy of oxygen vacancies can be decreased by as much as 0.25 eV upon application of an epitaxial strain of about +4% [4].

In this talk, I will present recent advancements on the microscopic characterization of oxygen vacancies in perovskite thin films by using computational first-principles methods. Specifically, I will show that vibrational phonons, namely, temperature-induced collective lattice excitations, play a crucial role on the strain-mediated control of defect chemistry in ABO_3 compounds [5]. Theoretical results will presented for archetypal systems $SrCoO_{3-\delta}$ [6] and $La_{1/2}Sr_{1/2}Mn_{1/2}Co_{1/2}O_{3-\delta}$, together with some insightful comparisons with recent experiments [7].

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[4] P. Agrawal et al., Phys. Rev. B 94, 104101 (2016)
[5] C. Cazorla, Phys. Rev. Appl. 7, 044025 (2017)
[6] P. Rivero and C. Cazorla, Phys. Chem. Chem. Phys. 18, 30686 (2016)
[7] S. Hu, Y. Wang, C. Cazorla, and J. Seidel, Chem. Mater. 29, 708 (2017)

Biography

Claudio Cazorla is an ARC Future Fellow in the School of Materials Science and Engineering in UNSW Sydney. Previously, he was a JAE-DOC Fellow in the Institute of Materials Science of Barcelona (Spain). His primary research interest is the application and development of computer simulation techniques to understand and predict new oxide-based and inorganic materials for nanoelectronics and energy applications.