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Interplay between structural complexity and magnetism in non-stoichiometric Pr2NiO(4+d) single crystals.

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Non-stoichiometric Pr2NiO(4+d) has emerged as a model system for its application as oxygen conductor in solid oxide fuel cells due to ambient oxygen conductivity, thermal stability at higher temperatures, large oxygen solubility range and a large fully-reversible oxygen uptake window. It is also thought that introduction of interstitial oxygen activates specific low-energy phonon modes that mediate oxygen transport at low temperatures.

Associated with oxygen intercalation in stoichiometric Pr2NiO4 is the emergence of structural complexity in the form of a well-defined and long-range ordered oxygen superstructure. Because of the convenience with which oxygen doping can be controlled in it, Pr2NiO(4+d) presents a system where we have the possibility to tailor the oxygen content and with that establish control over the resulting superstructure formation. The well-ordered superstructure indicates a correlation among the interstitial oxygen atoms which necessitates a deeper understanding of the role of electron density, Ni valence states and influence of the superstructure on the electronic properties of the compounds. We have made investigations on three different non-stoichiometric phases: Pr2NiO4.12, Pr2NiO4.25 and Pr1.5Sr0.5NiO4, which is isoelectronic to Pr2NiO4.25.

In this talk we discuss the interplay of structural complexity and its influence on valence states and magnetism in Pr2NiO(4+d), which can give a new insight into emergence of novel and interesting properties via hole-doping in the Ruddlesden-Popper phases. We also present the preliminary results of neutron scattering, neutron spectroscopy and macroscopic magnetic measurements made on the different non-stoichiometric phases of Pr2NiO(4+d).

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