Proposal Acronym	TEMPEST
Proposal Title:	Thermoelectricity in multifunctional perovskites
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Research area:	Physics PHY
Sub-discipline of research area:	Electronic properties of materials and transport
Category of research:	basic
Keywords:	Density functional theory, Thermoelectrics,Transport properties,Electronic structure, Semiconductors, Metals, Manganites, energy
Abstract:	High efficient Thermoelectric (TE) materials are important for power generation devices that are designed to convert heat to electricity and vice versa. The development of new types of TE materials with high performance is strongly driven by the need of sustainable and clean energy. In the present work we will study TE properties of perovskite manganese oxide (PMO) based multifunctional materials with a particular attention for calcium manganite CaMnO3. The thermoelectric properties will be analysed on the basis of electronic band structure, phonons and electron-phonon coupling properties. We will combine the well-known Boltzmann transport theory and the variational method with the predictive power of density functional calculations. Proposed project will prospect the possibility of perovskite oxides as multifunctional materials with broad spectrum of applications. For example, CaMnO3 so as to serve as the buffer layer for hybrid halide perovskite photovoltaic devices. The main reaso
Does this proposal possess any of the sensitive ethical issues detailed in ethical issues table?:	No