Minicolloque n° MMPS17 **x Oral** **☐ Poster**

Spin-polarized electronic states and atomic reconstructions at the antiperovskite Sr_3SnO(001) polar surfaces

R. Arras[a*], J. Gosteau[a], D. Huang[b], H. Nakamura[c], H. J. Zhao[c], C. Paillard[d] and L. Bellaiche[c]

a. CEMES, Université de Toulouse, CNRS, UPS, Toulouse, France
b. Max Planck Institute for Solid State Research, Stuttgart, Germany
c. Physics Department and Institute for Nanoscience and Engineering University of Arkansas, Fayetteville, Arkansas, USA
d. Laboratoire SPMS, CentraleSupélec/CNRS UMR8580, Université Paris-Saclay, Gif-sur-Yvette, France

* email : remi.arras@cemes.fr

First grown in 1980 [1], Sr_3SnO is an antiperovskite that shows good promise for fundamental research. It has been predicted to be a 3D Dirac semimetal with a band structure having 6 Dirac cones along the Γ-X directions [2]. This material is formally classified as a topological crystalline insulator [3], or as a higher-order topological insulator displaying hinge states [4]. Recently, superconducting behavior below a temperature $T \approx 5$ K has been evidenced in Sr-deficient Sr_3SnO antiperovskites [5] and some hints of a ferromagnetic ordering have been attributed to the possible presence of oxygen vacancies [6]. With formal oxidation states $[Sr^{2+}]_3Sn^{4-}O^{2-}$, this compound is expected to display an alternation of $(SrSn)^{2-}$ and $(Sr_2O)^{2+}$ polar atomic layers perpendicular to the [001] direction. It can thus be expected that growing Sr_3SnO (001) thin films could lead to electronic reconstructions, on the basis of a polar catastrophe scenario [7], or atomic reconstructions with the stabilization of structural defects such as vacancies. Due to the particular structure of antiperovskites and its predicted bulk band gap of a few tenths of meV, the properties of Sr_3SnO may be very sensitive to the growth conditions and to its stoichiometry.

We will present an *ab initio* study of the (001)-surface properties of the antiperovskite Sr_3SnO. We will first compare the relative energetical stability of different surface terminations, including possible atomic reconstructions induced by the presence of vacancies or adatoms. We will then describe their respective electronic structures and show how they could potentially lead to new ground states, including magnetic orderings or spin-orbit spin-splittings of the electronic states. Either conventional electronic reconstructions or magnetic transitions could have a decisive effect on the true realization of surface states in these compounds, and we thus expect our results to be useful for further experimental studies of this compound or other polar surfaces.

[1] A. Widera and H. Schäfer, Mater. Res. Bull. **15**, 1805 (1980).
[2] H. Nakamura, *et al.*, Nature Commun. **11**, 1161 (2020).
[3] T. H. Hsieh, *et al.*, Phys. Rev. B **90**, 081112 (2014). / C.-K. Chiu, *et al.*, Phys. Rev. B **95**, 035151 (2017).
[4] Y. Fang and J. Cano, Phys. Rev. B **101**, 245110 (2020).
[5] M. Oudah, *et al.*, Nature Commun. **7**, 13617 (2016).
[6] Y. F. Lee, *et al.*, Appl. Phys. Lett. **103**, 112101 (2013).
[7] J. Goniakowski, et al., Rep. Prog. Phys. **71**, 016501 (2007).

Acknowledgement:
This study has been partially supported through the EUR Grant NanoX No. ANR-17-EURE-0009 in the framework of the "Programme des Investissements d'Avenir". H.J., C.P. and L.B. thank the Vannevar Bush Faculty Fellowship (VBFF) from the Department of Defense. This work was granted access to the HPC resources of CALMIP (Allocation No. 2020-2021/P1229).