Ruthenium oxides peculiarities probed by the Seebeck effect and prospection of novel thermoelectric chalcogenide materials assisted by machine-learning

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In metallic ruthenium oxides, transport coefficients such as the Seebeck effect S can be described considering a coexistence of metallic carriers together with localized magnetic moment contributions enhancing S[1]. The aim of this work was to investigate the Seebeck coefficient in several ruthenium oxides presenting different electronic and magnetic backgrounds to better understand this coexistence effect. Different structures have been investigated: rutile, hollandites[2], R-type ferrites[3] and perovskites. These results have been compared to well known $SrRuO_3$ and Sr_2RuO_4 and provide evidence of high T Seebeck coefficient protected from band structure considerations in ruthenium oxides.
Optimization of chemical composition or process for substituted-GeTe using active learning assisted by machine learning and Bayesian optimization[4, 5]. Random Forest algorithm based on elementary descriptors only has demonstrated relatively good performances in modeling the thermoelectric properties for ternary and quaternary substituted-GeTe and also for Cu_2ZnSnS_4 Kesterite. Prediction for proposed chemical compositions or process parameters targeting optimized thermoelectric properties.

[1] I. Terasaki, Y. Sasago and K. Uchinokura, Phys. Rev. B **56**, R12685 (1997).
[2] F. Pawula, S. Hébert, D. Pelloquin, and A. Maignan, J. Mater. Chem. C **7**, 235106 (2021).
[3] F. Pawula, R. Daou, S. Hébert, D. Pelloquin, J. Juraszek, and A. Maignan, Phys. Rev. B **103**, 235106 (2021).
[4] A. S. Nugraha, G. Lambard, J. Na, M. S. A. Hossain, T. Asahi, W. Chaikittisilp, and Y. Yamauchi, J. Mater. Chem. A **8**, 13532 (2020).
[5] G. Lambard, T. T. Sasaki, K. Sodeyama, T. Ohkubo, and K. Hono, Scr. Mater. **209** 114341 (2022).