Tackling the Complexity of Multi-Component Oxide Surfaces

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Multicomponent oxides are Physics-rich, versatile materials used in a variety of applications, including energy production, spintronics, and catalysis. Their surfaces are crucial to their functionality in applications, yet they are scarcely investigated. As a result, most computational studies assume bulk-truncated surface terminations. Our atomically resolved studies in ultra-high vacuum, however, show that this rarely reflects reality [1–3].

Here, I will use the example of lanthanum-strontium manganite (LSMO) to show the variety of complex surface reconstructions that multicomponent oxides can display as a function of their composition. I will especially focus on how we managed to organize the complexity by constructing an experimental surface phase diagram.

Identifying and organizing structures is only the first step, though. A deeper understanding can only be achieved when structural models for the measured surface reconstructions are available. However, the intrinsic complexity of the problem poses great challenges in this respect. In the second part of the talk, I will discuss how a nearly forgotten but powerful experimental technique, LEED-*I*(*V*), can provide substantial help to solve such a complex problem. I will discuss our recent developments of software and hardware infrastructure for revitalizing the LEED-*I*(*V*) technique.

References

[1] G. Franceschi, *et al.*, Phys. Rev. Mater. **5**, L092401 (2021).
[2] G. Franceschi, *et al.*, J. Mater. Chem. A **8**, 22947 (2020).
[3] M. Riva, *et al.*, Phys. Rev. Mater. **3**, 043802 (2019).