Title: **Charge-order-driven ferroelectricity in perovskite superlattices from first principles**

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Abstract:

The application of first-principles methods to the systematic study of families of materials opens up new avenues to the theoretical design of materials with targeted functional properties. In this talk, I will discuss recent work on the systematic study of selected families of perovskite superlattices, including structure determination and investigation of charge disproportionation and charge ordering, magnetic ordering and Jahn-Teller distortions. The resulting identification of the 1:1 LaVO3/SrVO3 superlattice as a candidate charge-order-driven ferroelectric, and novel aspects of the electric polarization in this electronic ferroelectric, will be presented and discussed.