

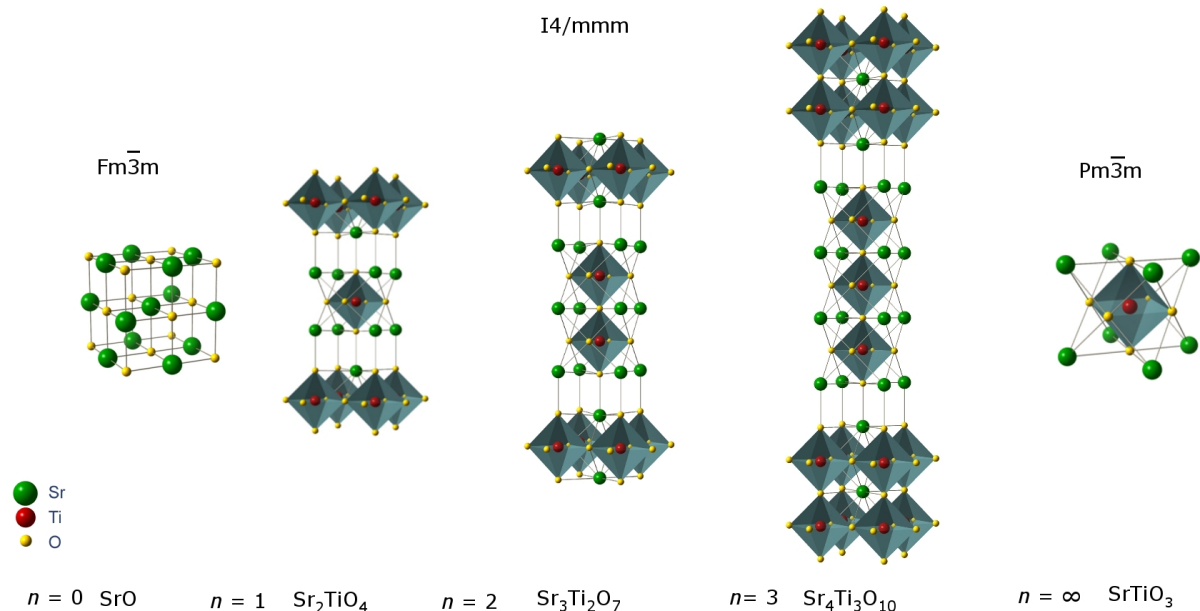
# Electronic structure of the homologous series of Ruddlesden-Popper phases $\text{SrO}(\text{SrTiO}_3)_n$ , ( $n = 0 - 3, \infty$ )

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The system  $\text{SrO}(\text{SrTiO}_3)_n$ , shown in Figure 1, contains promising compounds for several applications, including tunable microwave components for communication and radar applications as well as alternative gate oxides for tunable dielectric devices and as photocatalysts, whose functionalities all depend in particular on the band structure of the respective crystal. While the electronic structure of  $\text{SrO}$  and  $\text{SrTiO}_3$  is sufficiently clarified in literature, there is a lack of information concerning the Ruddlesden-Popper (RP) phases. In this work density functional theory is used to compute the electronic structure for the homologous series with  $n = 0 - 3, \infty$ . The according band structures are presented and effective masses are given for the complete system. In addition, the calculations are consulted to discuss the thermodynamical stability of the RP phases, confirming the gain of formation energy up to  $n = 3$  as reported in recent literature. A promising possibility for applications has been found, analyzing these band structures: As the optical gaps at distinct high-symmetry points of the Brillouin zone show different dependencies on the lattice parameters, as it is reported for  $\text{SrO}$  in literature, a similar behavior could be expected in particular for the RP phase with  $n = 1$ .



**Fig 1:** Homologous series of Rudlesden-Popper phases  $\text{SrO}(\text{SrTiO}_3)_n$  from  $n = 0$  to  $n = 3, \infty$ .

The authors acknowledge funding by the DFG within the project DFG 409743569, ZS 120/1-1. Further funding was provided within DFG 442646446, ZS 120/5-1.