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Electronic structure of the homologous series of Ruddlesden-Popper phases SrO(SrTiO3)□, (□= 0 - 3, ∞)

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While the electronic structure of SrO and SrTiO3 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 □ = 0 - 3, ∞. 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.

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