TECHNISCHE UNIVERSITÄT BERGAKADEMIE FREIBERG

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ELECTRONIC STRUCTURE OF THE HOMOLOGOUS SERIES OF RUDDLESDEN – POPPER PHASES IN STRONTIUM TITANATE

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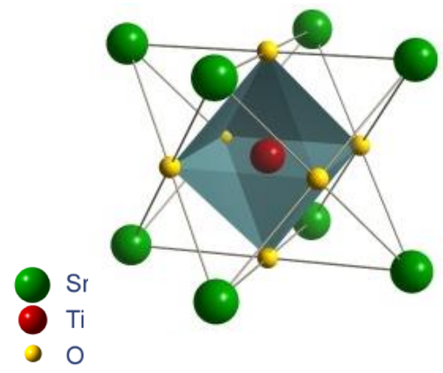
Motivation

The system $SrO(SrTiO_3)_n$ contains promising compounds for several applications, among them:

- Substrate Material
- Alternative gate oxide for tunable dielectric devices
- Photocatalyst
- All-in-one rechargeable energy storage
- Resistance switching random access memory (RRAM)

Features depend on the electronic structure
Electronic structure of SrO and $SrTiO_3$ well known
Lack of information concerning the Ruddlesden – Popper (RP) phases

Strontium Titanate

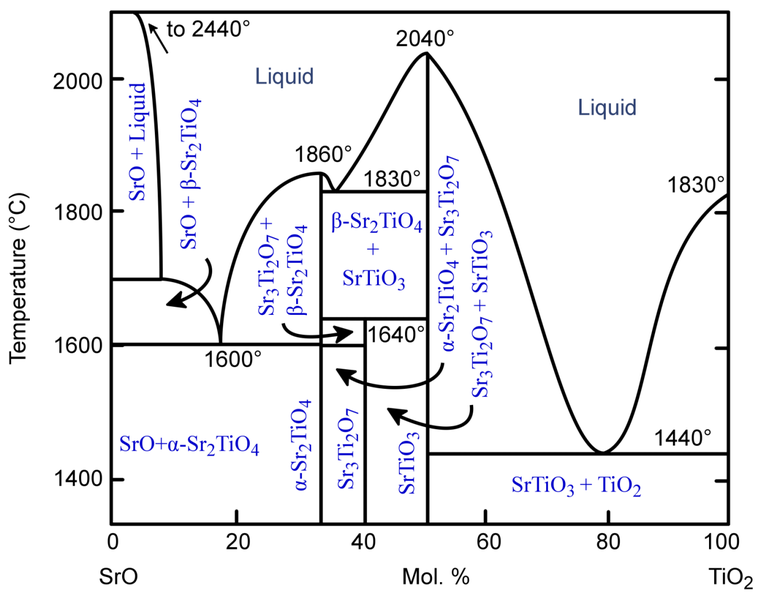


Perovskite structure:

ABO_3
Sr^{2+} cuboctahedral
Ti^{4+} octahedral
O^{2-}

Lattice parameter: 3.905 Å
Space group: $Pm\bar{3}m$

The System $SrO(SrTiO_3)_n$



Quasi-binary phase diagram SrO –TiO_2 [1]

Compositional boundaries:

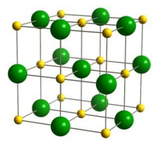
•SrO	mol% = 0	$n = 0$
•$SrTiO_3$	mol% = 50	$n = \infty$

Intermediate Phases:
Ruddlesden – Popper

•Sr_2TiO_4	$n = 1$
•$Sr_3Ti_2O_7$	$n = 2$
•$Sr_4Ti_3O_{10}$	$n = 3$

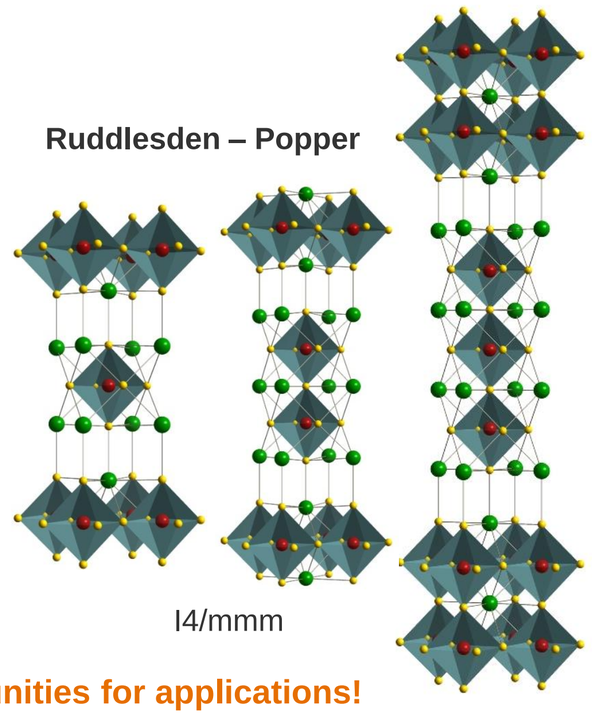
Introduction of SrO layers as ordered SrO – OSr stacking faults

SrO



$Fm\bar{3}m$

Ruddlesden – Popper



I4/mmm

→New electronic structure, properties & opportunities for applications!

Density Functional Theory

ABINIT code
Pseudopotentials
Local density approximation (LDA)
Broyden – Fletcher – Goldfarb – Shanno minimization (BFGS)

initial parameters → SCF * → atomic relaxation → SCF * → DOS & bandstructure

**Self consistent field*

Stability of RP Phases

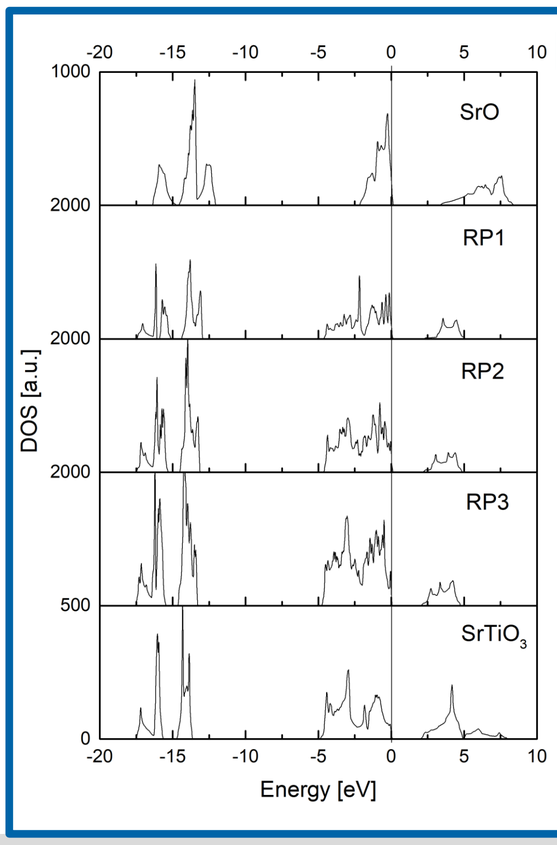
Energy of formation compared to the presence of SrO & $SrTiO_3$

→ $E_f^{RPn} = E[SrO(SrTiO_3)_n] - n \cdot E[SrTiO_3] - E[SrO]$

- Sr_2TiO_4 $E_f^{RP1} = -0{,}1493$
- $Sr_3Ti_2O_7$ $E_f^{RP2} = -0{,}2003$
- $Sr_4Ti_3O_{10}$ $E_f^{RP3} = -0{,}2113$

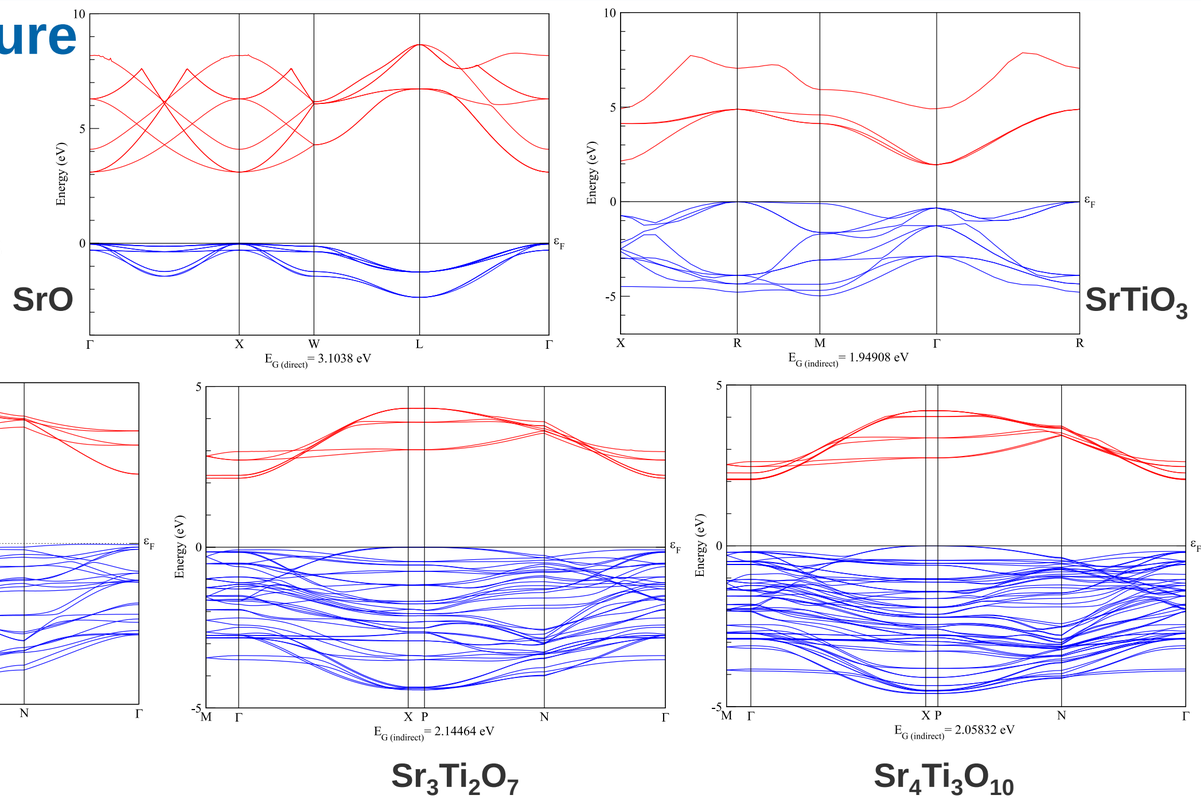
→ RP phases *n* = 1 – 3 are energetically favored!

Electronic Structure



Trends in ascending series:

- SrO character decreases
- $SrTiO_3$ character increases
- Bandgap decreases



[1] Redrawn from: R. C. Ropp, Encyclopedia of the alkaline earth compounds (Elsevier, Oxford, 2013)

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