

Funkcionālie materiāli rezistīvai pārslēgšanas atmiņai (MATERA)

J. Purāns, E. A. Kotomins,
R. I. Eglītis, A. Kuzmins,
R. Kalendarevs, A. Popovs
2009. gada rezultāti

Galvenie teorijas mērķi:

Aprēķini no pirmajiem principiem priekš pamata defektiem kuri ir svarīgi priekš rezistīvās pārslēgšanas dopētā SrTiO_3 :

-- Fe, Nb, un O vakances

Teorētiskā metode: programma CRYSTAL kombinēta ar periodisku modeli, izmantojot LASC paralēlo kompjūteru

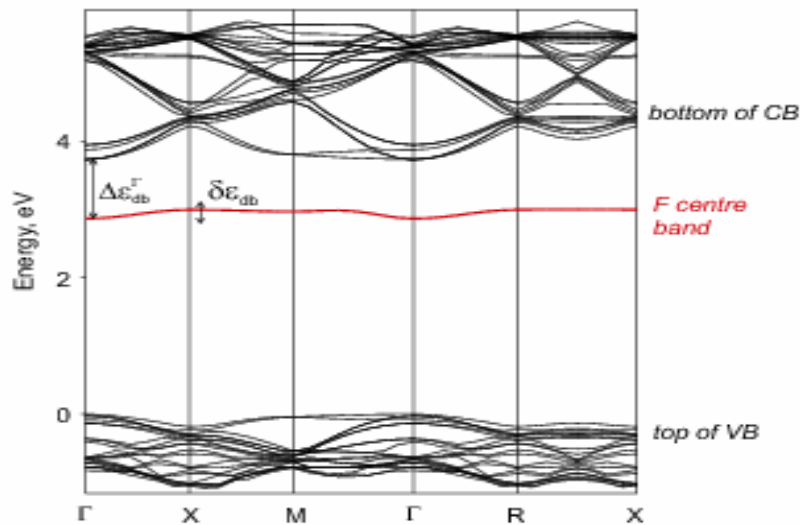
Galvenie rezultāti ir publicēti **European Physical Journal B**, 2009, **73**, p.53-57.

First-principles study of bulk and surface oxygen vacancies in SrTiO₃ crystal

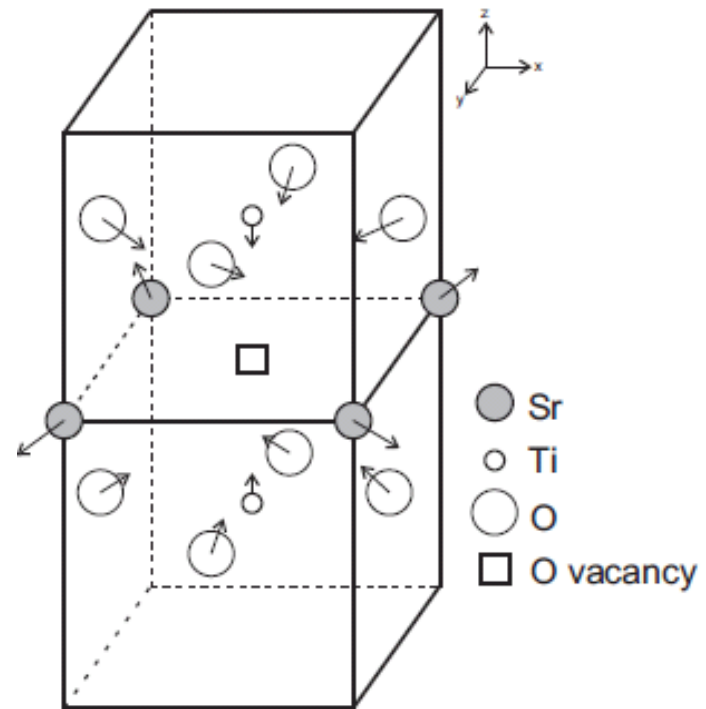
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- **R.I. Eglitis, E.A. Kotomin, tiks iesniegts, 2009**

Band structure calculations and position of the bulk and surface V_o (F center) energy bands



Shallow defect levels,
easy ionization and metallization
at higher defect concentrations



Local atomic relaxation

***Paper 2: Ab initio* calculations of Nb doped SrTiO₃**

R. I. Eglitis and E. A. Kotomin, in preparation

3 x 3 x 3 expanded unit cell → 135 atoms

→ relatively low 4% Nb doping

Nb replaces Ti and expands the lattice by 0.05 Å

The effective charges (Sr=+1.923e; Ti=+2.772e; O=-1.569e; Nb=3.13e) reveal Ti-O bond covalency (+64 me) is considerably larger than Nb-O (+8 me) because Nb ion is more ionic

Nb is also a shallow donor in SrTiO₃

Main conclusions

- Shallow donor (bulk and surface) vacancy defects, easy material metallization even at moderate vacancy concentrations
- Large segregation trend predicted for both neutral and even more for charged vacancies (F and F⁺ centers)
- F⁺ centers are deeper than neutral F centers
- Nb impurity produces also shallow donor levels even at low concentration

Future work (2010):

- Charged Fe(3+) impurities:
their complexes with oxygen vacancies
in the bulk and at the surface
- Charged Fe(3+) segregation towards surface
- verification of models developed in EXAFS experiments