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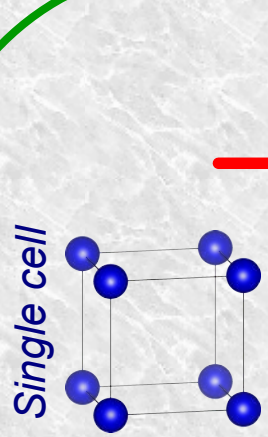
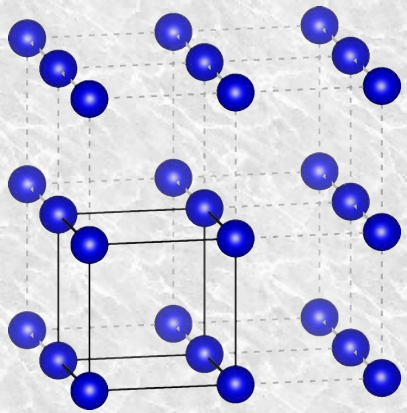
Electronic structure and magnetic properties of low-dimensional nonstoichiometric rutile

From supercell to CPA



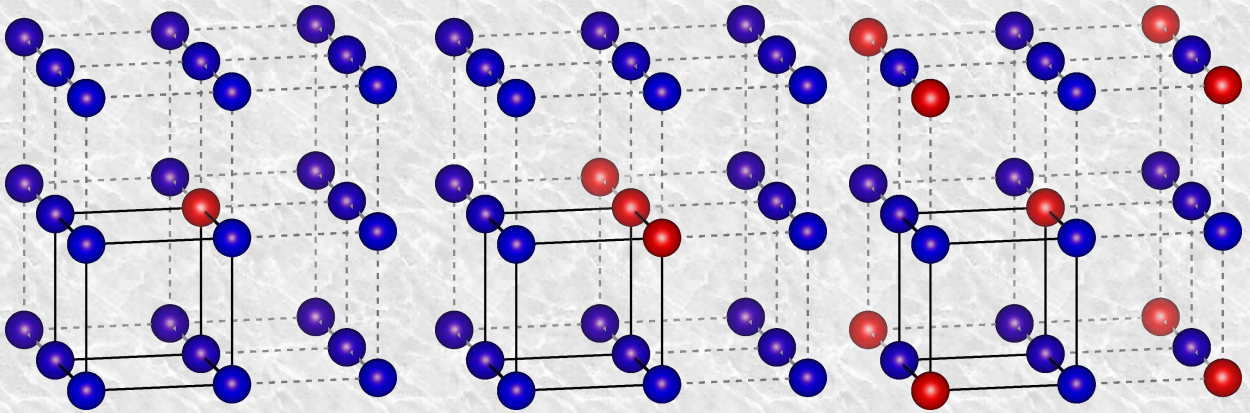
Single cell



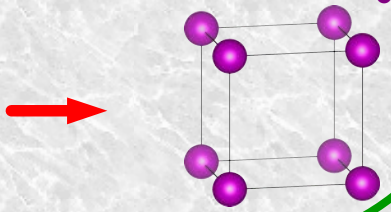
Supercell

Supercell with doubled impurity concentration

Or such impurity positions in the same supercell?

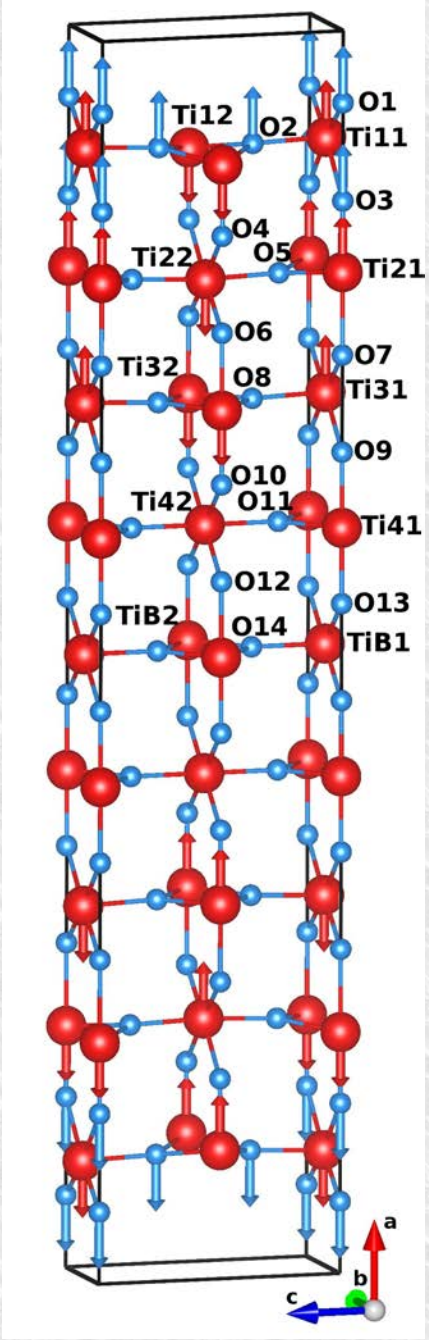


Supercell with single impurity

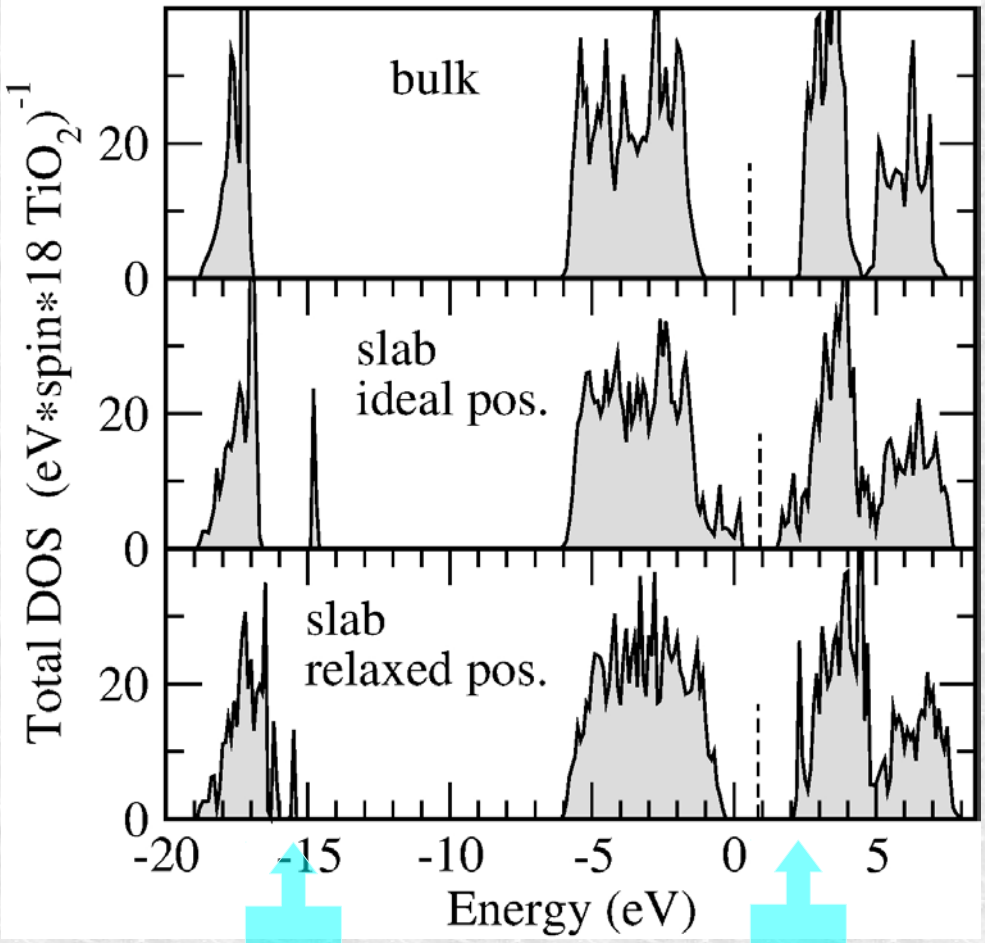


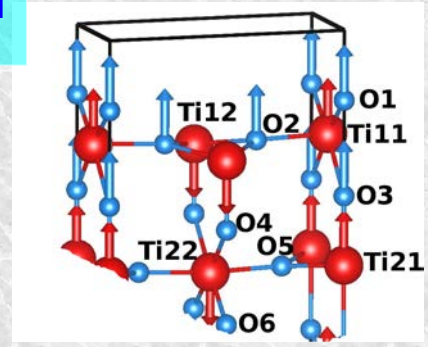
Single cell of effective atoms

Structural model for 2D TiO_2 rutile unit cell



Stoichiometric 3D versus 2D TiO_2





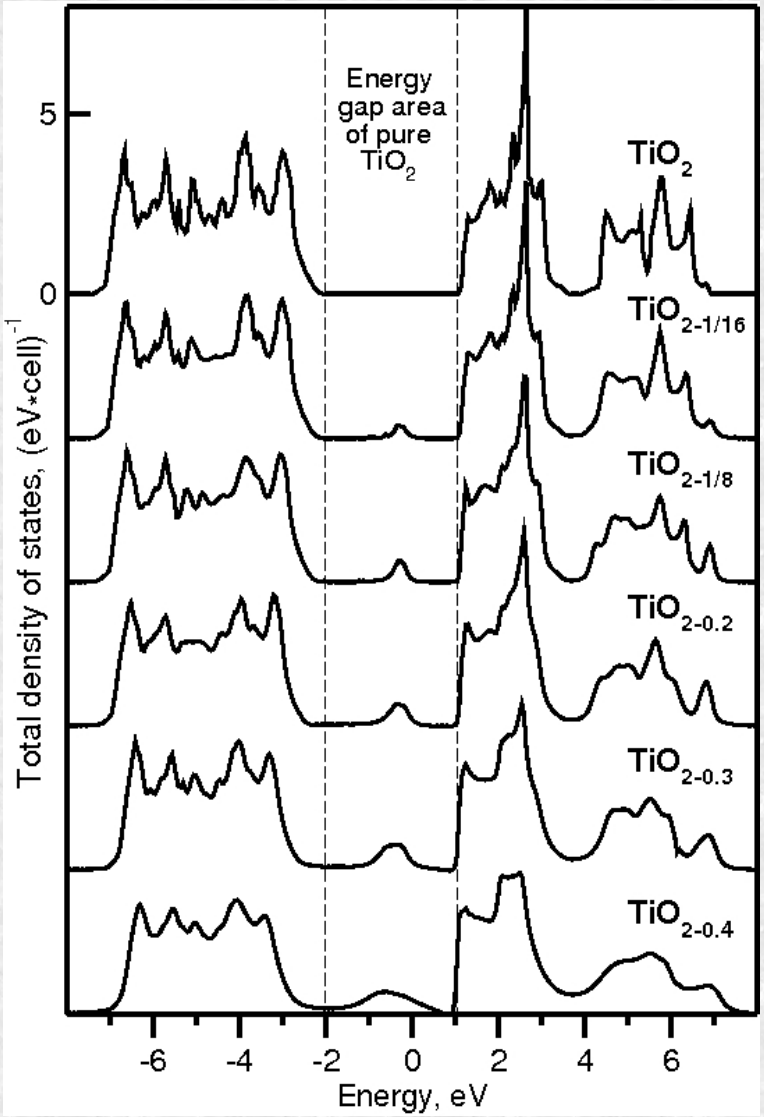
Electronic structure of

3D TiO_2 (upper panel),

2D TiO_2
without (middle panel) and with (lower panel) taking into account the atomic displacements.

Fermi levels indicated with vertical dashed lines are placed in the band gap centers.

3D $TiO_{2-\delta}$

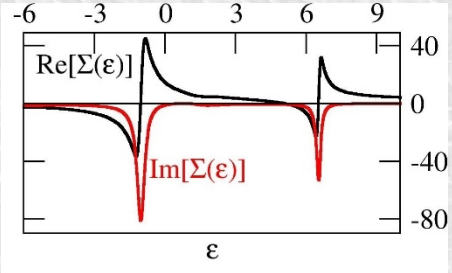


DOS evolution in dependence on nonstoichiometry in oxygen sublattice.

In the energy gap of pure TiO_2 the "vacancy" peak appears, growths in height and broads in width with the increase of δ .

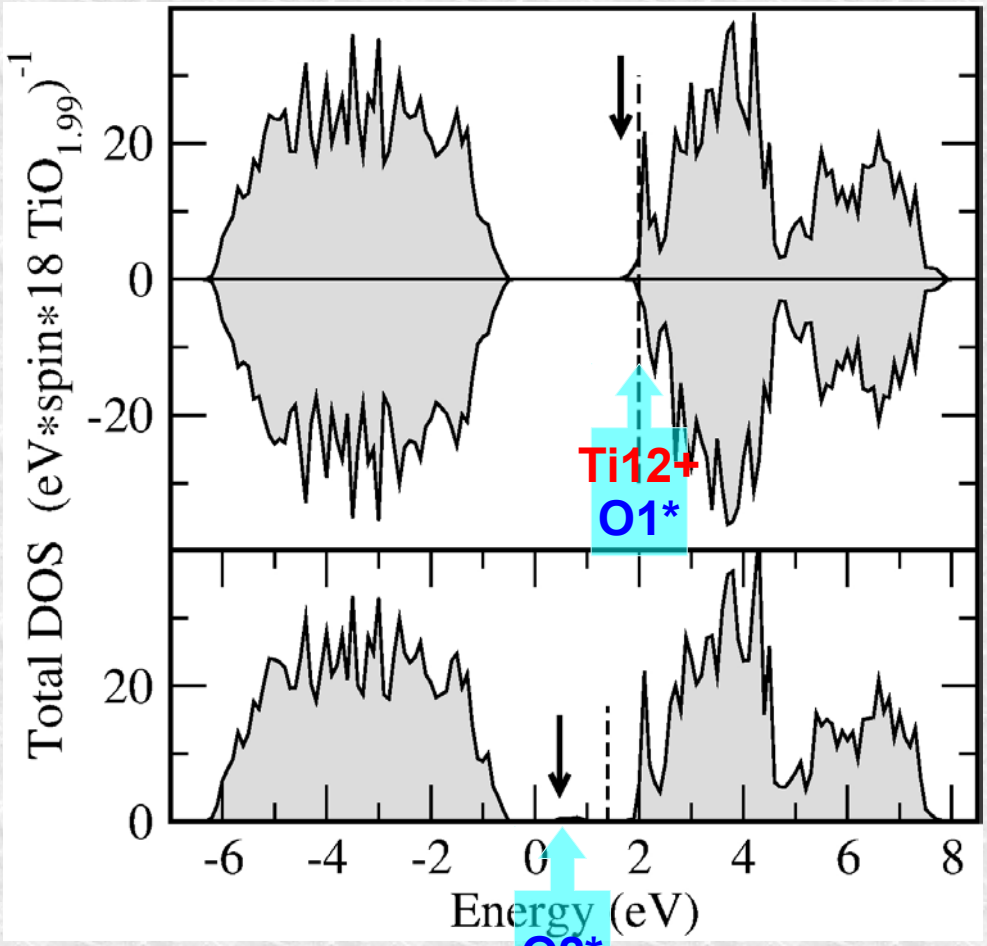
This peak has *s* symmetry (originated from O 2s-states), but has O 2*p*- *и* Ti 3*d*-states contributions also.

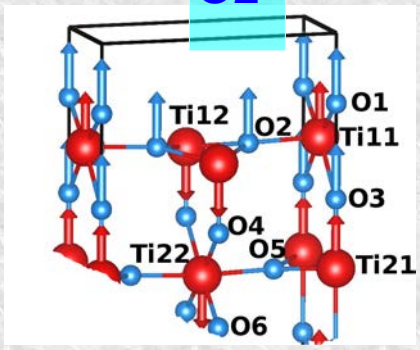
Energy position of this peak coincides with infra-red absorption and ultra-violet emission experimental data.



Self-consistent coherent potential of s-states of effective oxygen site for $TiO_{2-\delta}$.

Nonstoichiometric 2D $TiO_{1.99}$





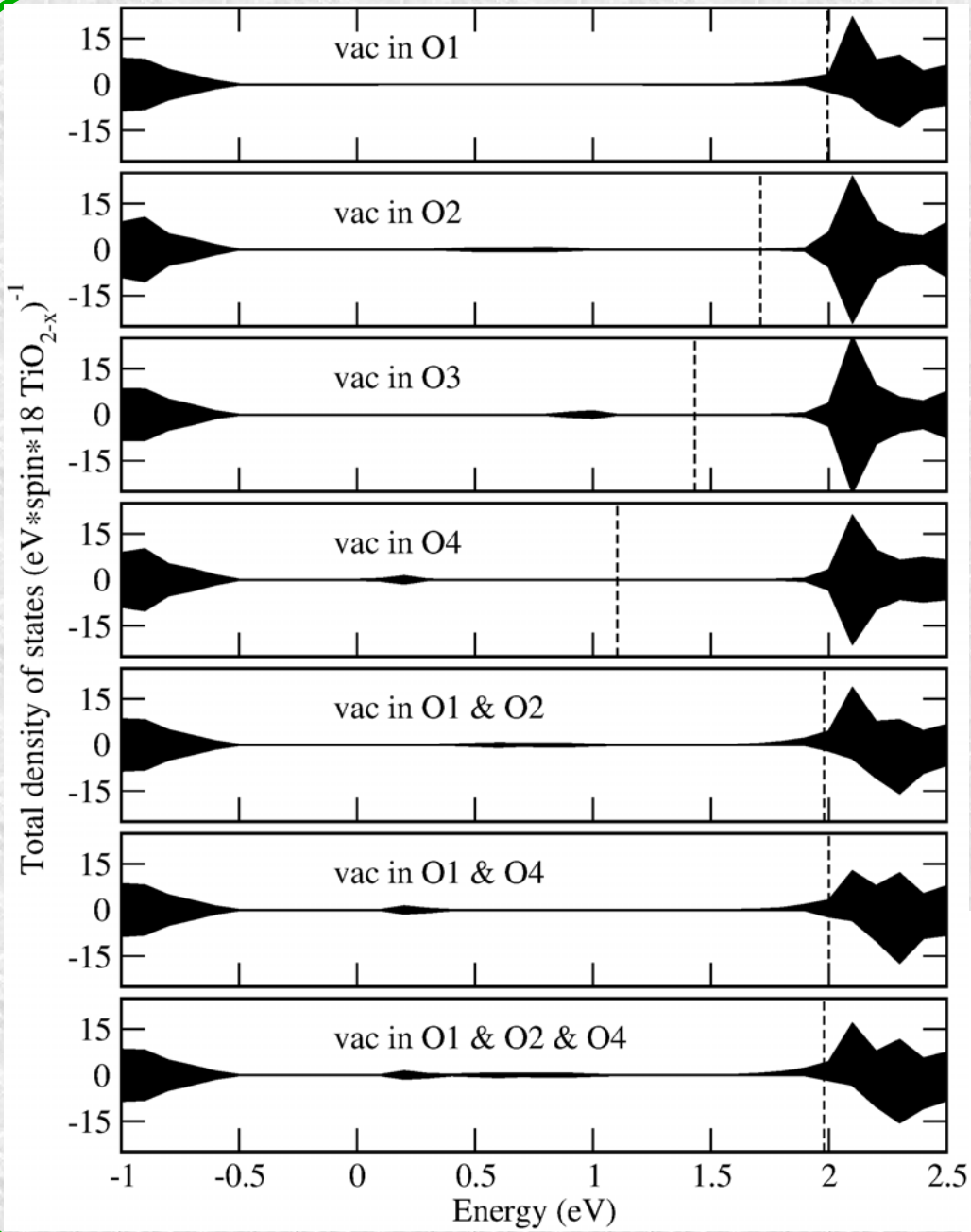
Electronic structure of 2D $TiO_{1.99}$ with vacancies in the O1 (upper panel) and

O2 (lower panel) sublattices.

The arrows indicate the positions of the vacancy states.

The Fermi level is indicated with the vertical dashed line.

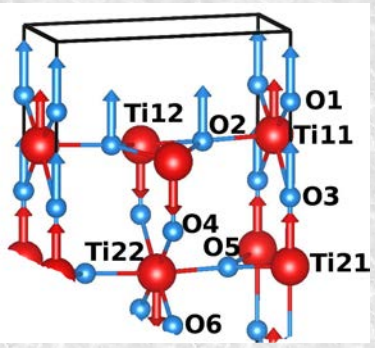
Vacancies in different oxygen sublattices



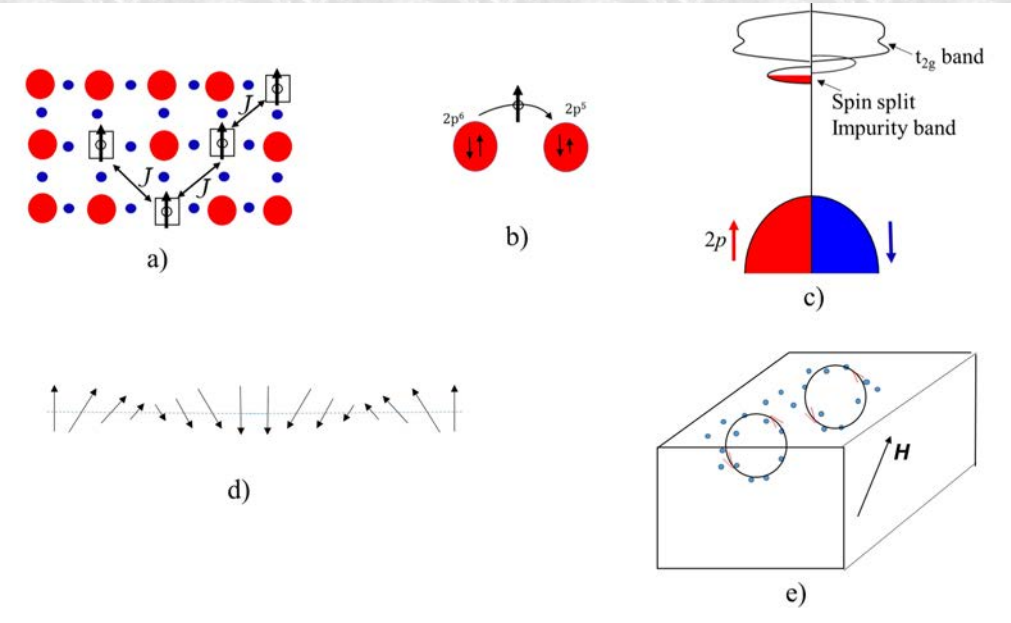
Electronic structure of 2D TiO_{2-x} with vacancies in different oxygen sublattices in narrow energy window around the Fermi level.

For upper 4 panels the composition is $TiO_{1.99}$, for the next 2 panels – $TiO_{1.98}$, for the bottom panel – $TiO_{1.97}$.

The Fermi level is indicated with the vertical dashed line.



Appropriate models for surface magnetism



J M D Coey *et al.*, J. Phys.: Condens. Matter **28** (2016) 485001.

Models explaining the magnetism originating from the surface:

(a) Conventional Heisenberg ferromagnetism due to localized electrons with s = 1⁄2 situated near oxygen defects;

(b) Zener ferromagnetism of 2p oxygen holes;

(c) Stoner ferromagnetism of electrons in a defect-related impurity band;

(d) Magnetism associated with a noncollinear spin texture;

(e) Giant orbital paramagnetism associated with surface currents.

Conclusions

- Coherent potential approximation is applied to study the electronic structure and magnetic properties of $TiO_{1.99}$ rutile (110) surface.
- Stoichiometric 2D TiO_2 is found to be a nonmagnetic semiconductor.
- Oxygen vacancies on the surface lead to metallic type of the electronic spectrum.
- Additionally, they result in the appearance of spin magnetic moments on Ti atoms surrounded by only five oxygen atoms.
- The vacancies in all the other oxygen positions except the surface do not change nonmagnetic semiconducting character of 2D $TiO_{1.99}$.
- Stoner ferromagnetism of a defect related impurity band is the mechanism for the formation of d-Ti spin magnetic moments.

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- References:
  see http://michael.korotin.name