Local structure and superconductivity in BiS_2-based materials

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Società Italiana di Fisica, 101° Congresso nazionale

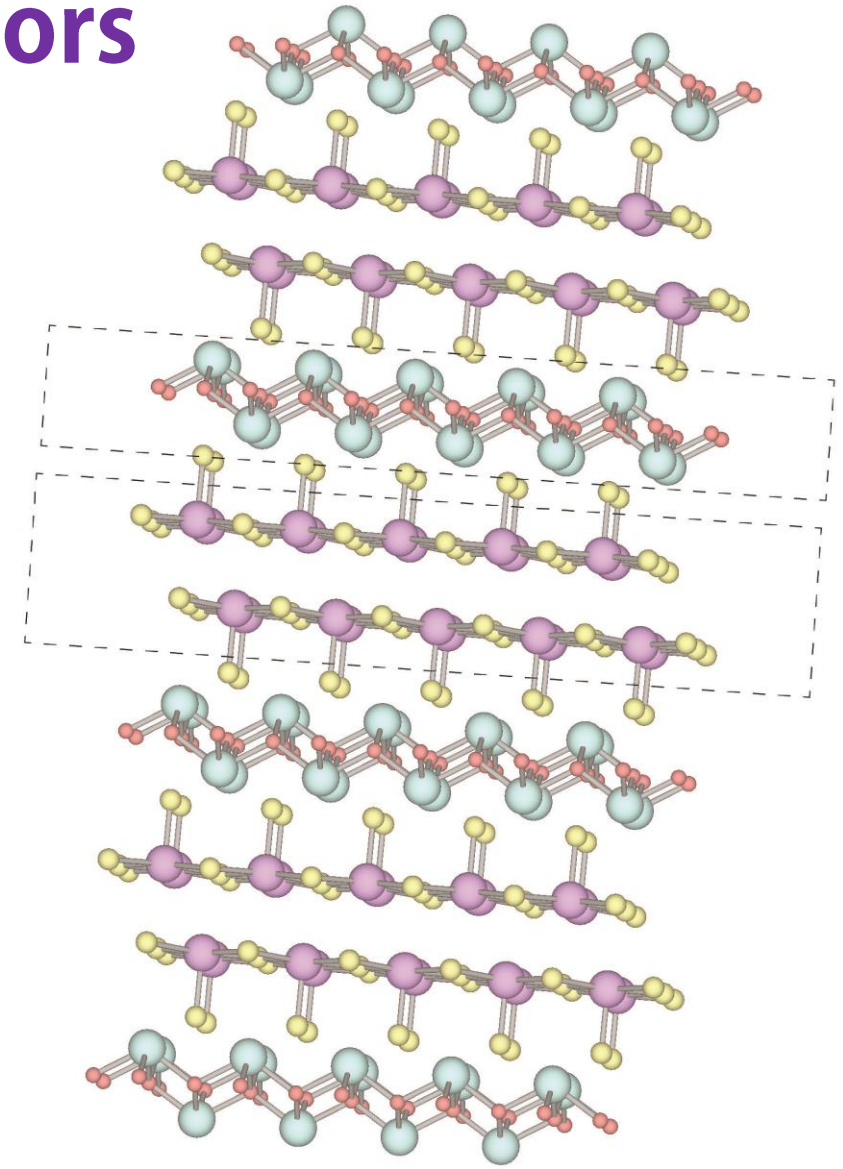
Roma, 21-25 Settembre 2015

The physics of layered superconductors

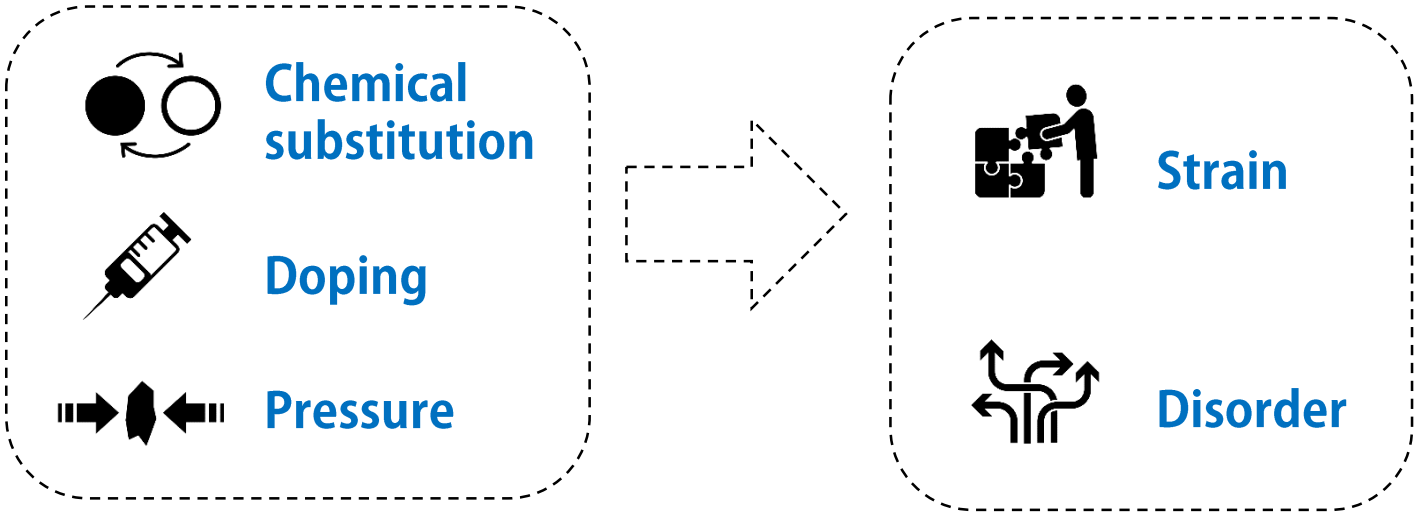
Nearly-2D materials

Large fluctuation in different degrees of freedom

Susceptibility to external perturbations

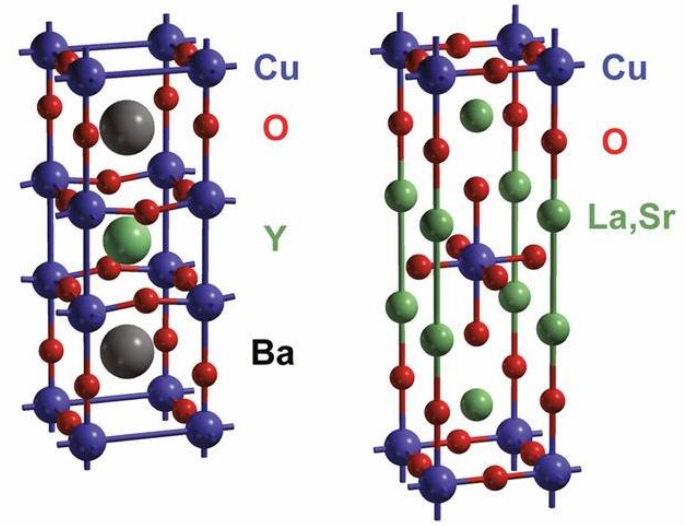


What determines the physical properties?



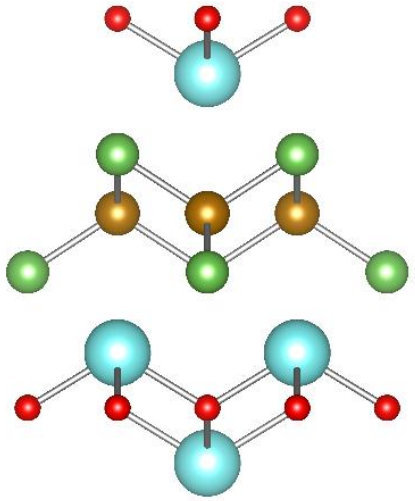
A new family of layered superconductors

HighTc superconductors



123,2201,2212,2223,....

Fe-based compounds



1111,11,112,122,1048...

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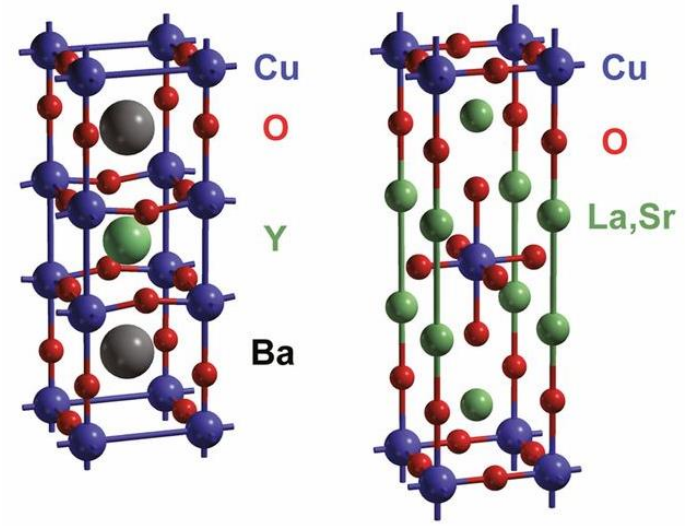

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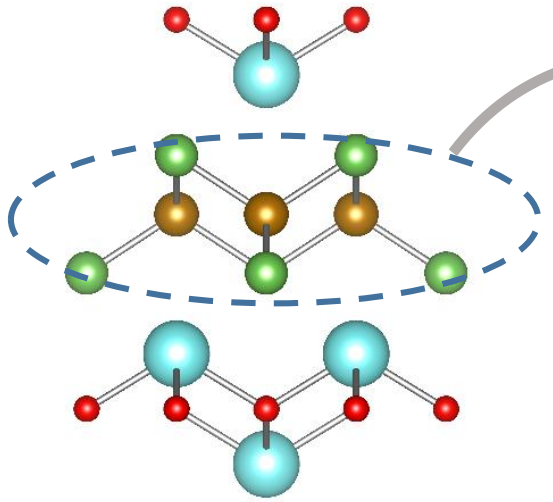
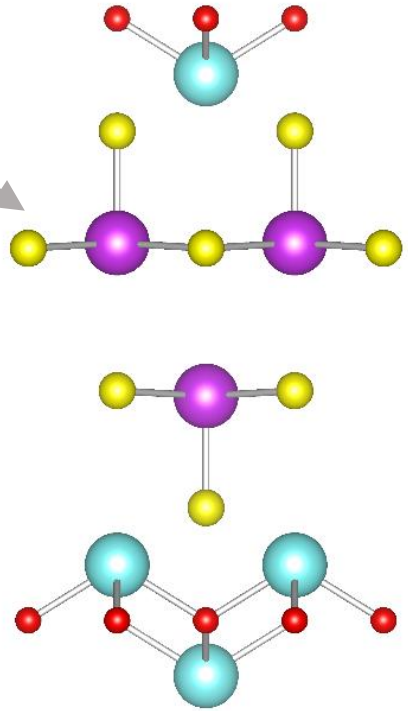


1111,11,112,122,1048...

New BiS_2-based materials



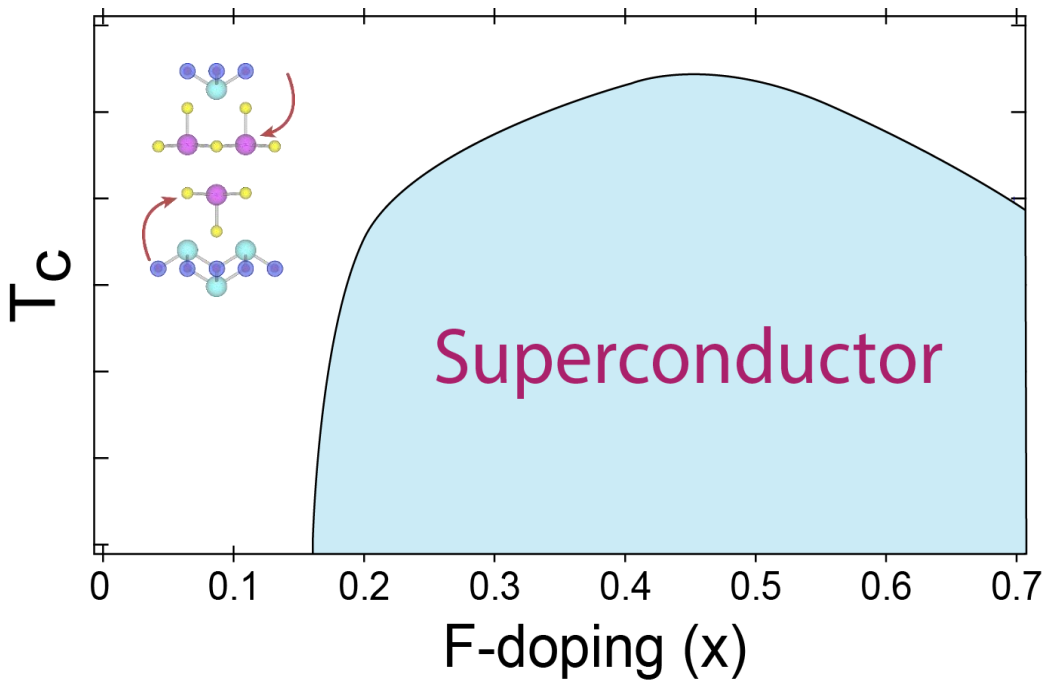
$REOBiS_2$

Y. Mizuguchi et al, PRB 86 220510 (R) (2012)

BiS_2-based superconductor family

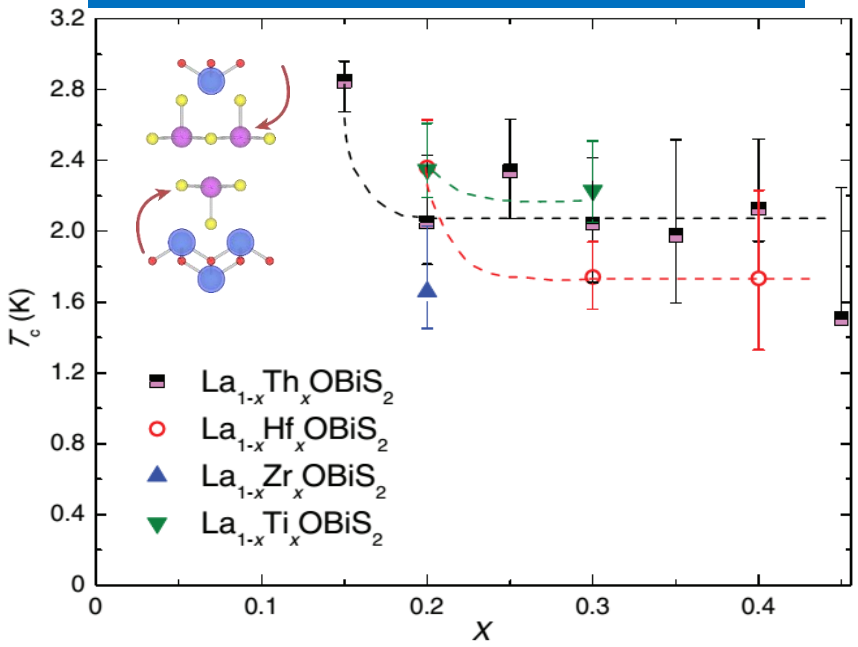
How to trigger SC in $REOBiS_2$

Partial substitution of O^{2-} by F^-



	Tc
$LaO_{1-x}F_xBiS_2$	2.8 K
$CeO_{1-x}F_xBiS_2$	3.0 K
$PrO_{1-x}F_xBiS_2$	3.5 K
$NdO_{1-x}F_xBiS_2$	4.0 K

Substitution of RE^{3+} with RE^{4+}

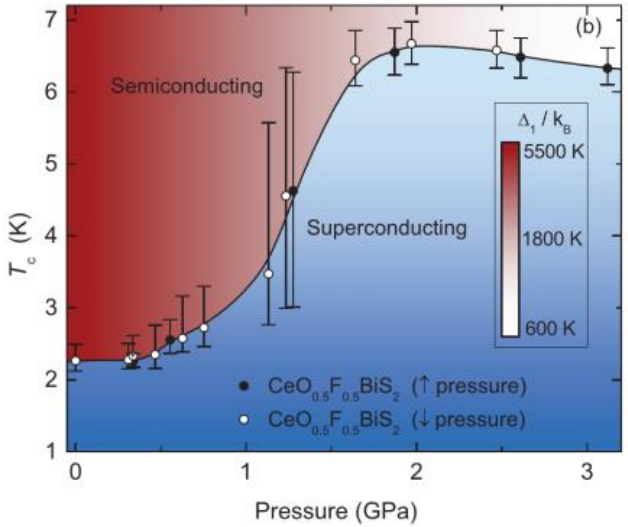


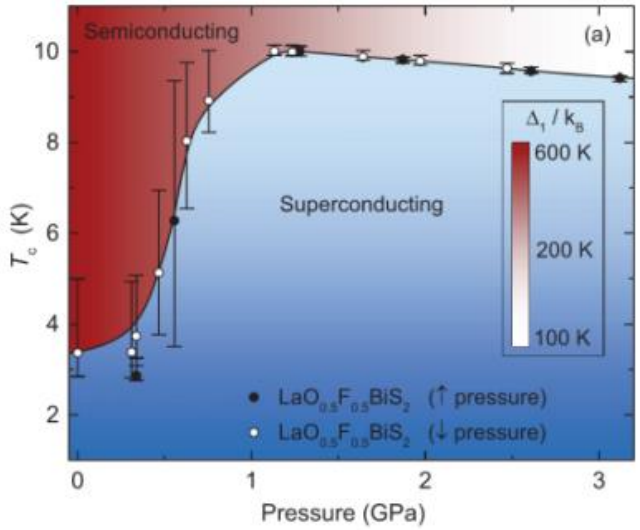
? **F-doping... Adding carriers and/or optimizing the lattice (?)**

BiS_2-based superconductor family

Pressure enhanced SC in $REOBiS_2$

	Tc	New Tc
$LaO_{1-x}F_xBiS_2$	2.8 K	10 K
$CeO_{1-x}F_xBiS_2$	3.0 K	7 K
$PrO_{1-x}F_xBiS_2$	3.5 K	11 K
$NdO_{1-x}F_xBiS_2$	4.0 K	6 K



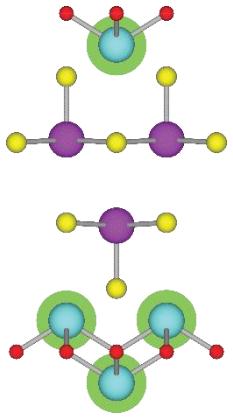


C.T. Wolowiec et al, PRB 88 064503 (2013)

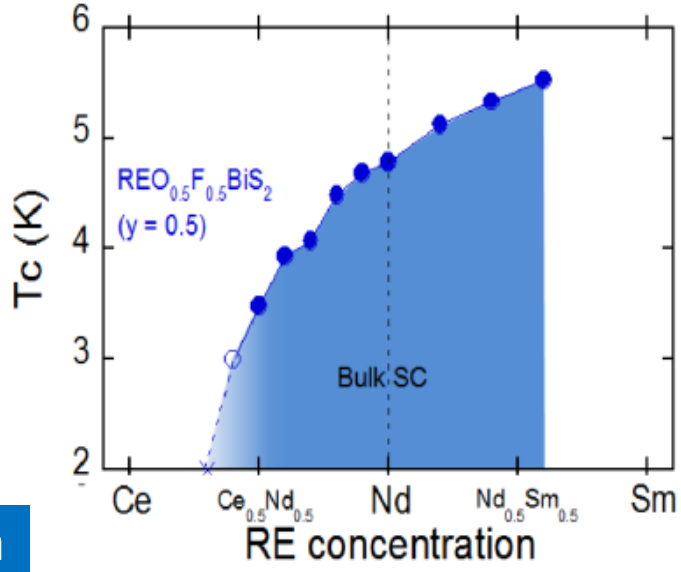
Similar effects has been obtained from high-pressure annealing techniques

BiS_2-based superconductor family

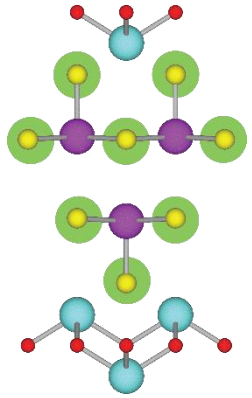
Effect of chemical pressure in $REOBiS_2$

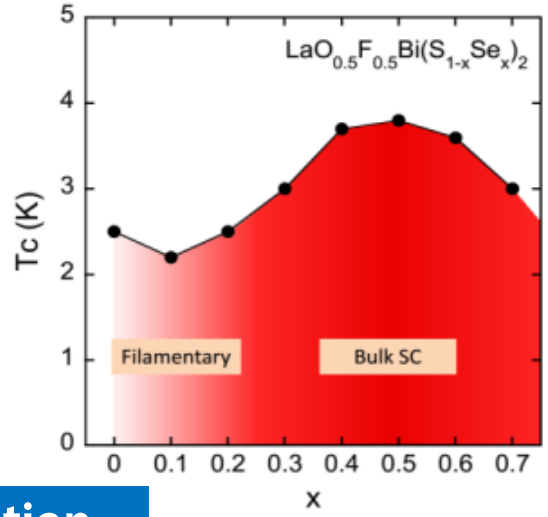


RE-substitution



J. Kajitani et al, Physica C 504 33 (2014)





$S_{1-x}Se_x$ substitution

What matters for superconductivity?

(non) conventional ?

BiS_2-based share many features with Fe-based

- Multiband superconductivity
- Coexistence of superconductivity and magnetism
- Layered structure
- Huge pressure/HP annealing/chemical pressure effects
- Fermi Surface nesting
- **Importance of local lattice structure**

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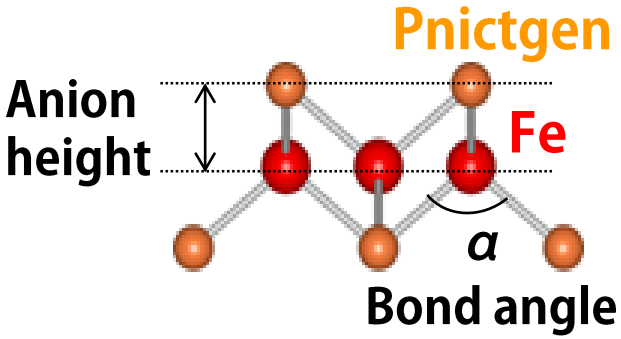
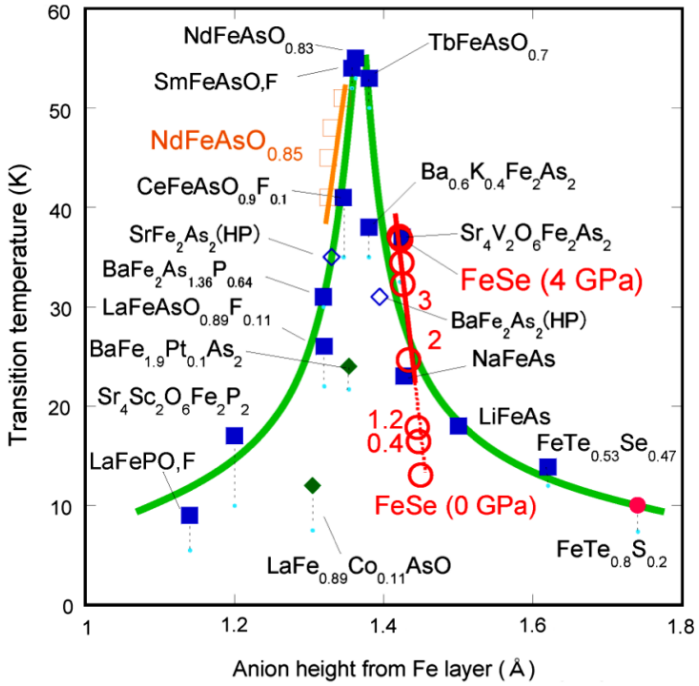
Structural order parameters in Fe-based compounds





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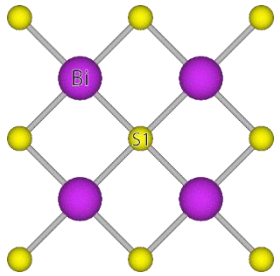
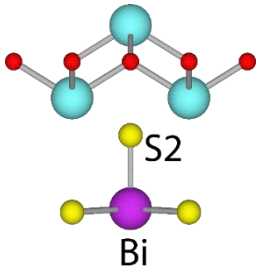
Search for a local order parameters in BiS_2-based materials



In-plane Bi-S bond?

T. Yildrim, PRB 87 020506 (R) (2013)



Out-of-plane Bi-S bond?

Interlayer distance?

H. Usui et al, PRB 86 220501 (R) (2012)
K. Suzuki et al, Phys. Proc. 45 21 (2013)

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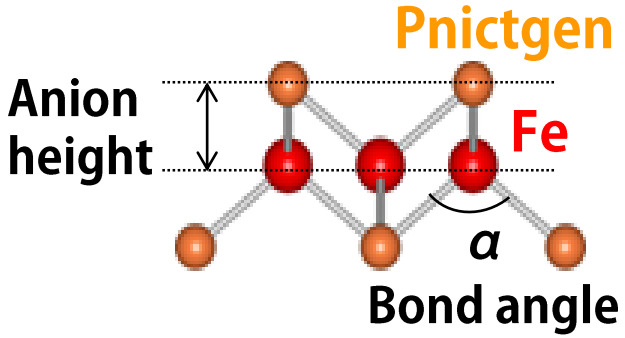
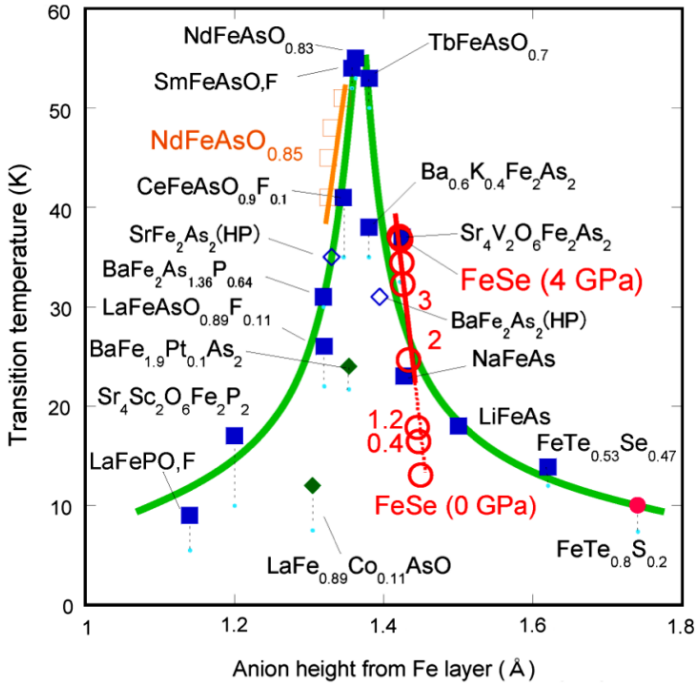
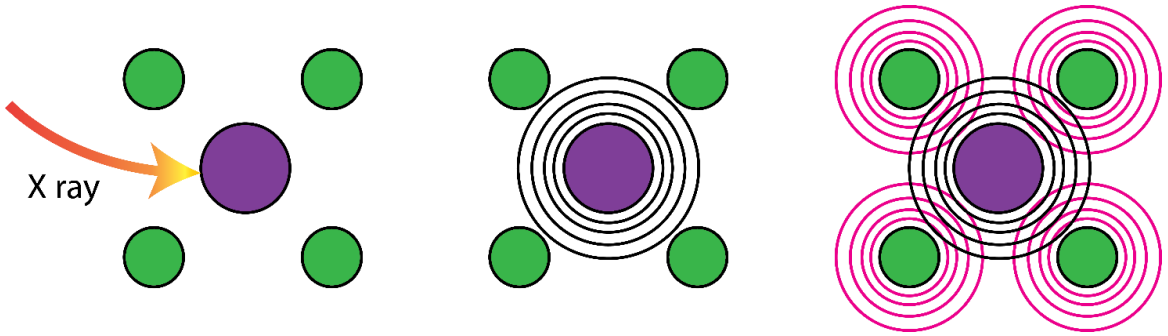
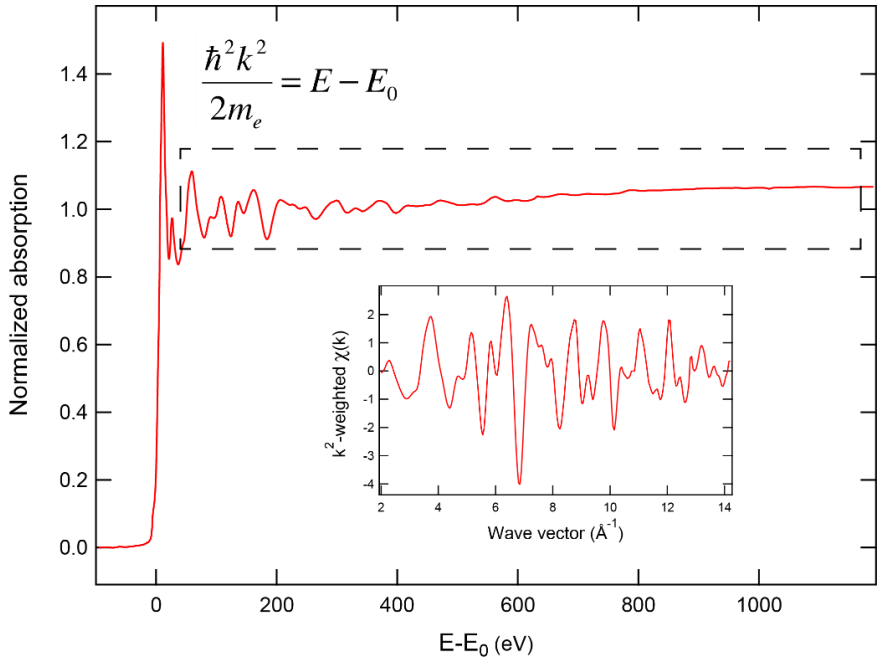




How to observe local lattice distortions in solid state?

Extended X-ray absorption fine structure (EXAFS) spectroscopy





Element selective - absorption edge is a fingerprint

Local coordination sensitive - probing <10 Angstrom from absorber

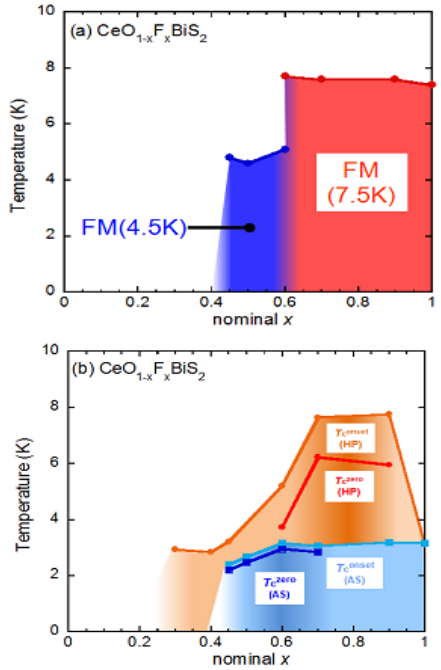
Bulk sensitive - information depth > 10 micron

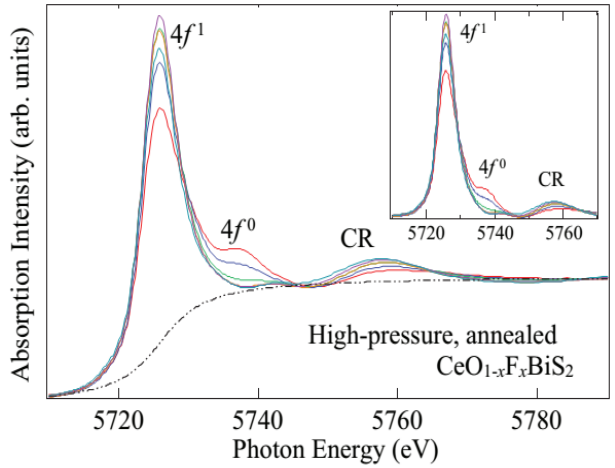
$$\chi(k) \propto \sum_i N_i \int g(r) F(k,r) \sin(2kr + \phi_{ci}) dr$$

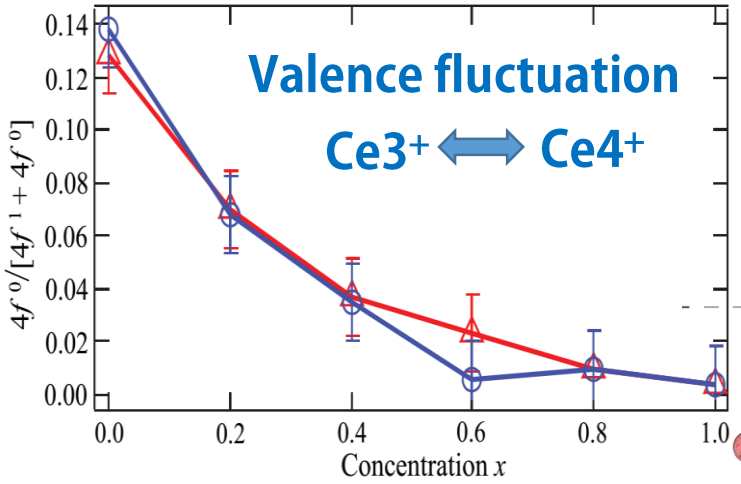
Local effect of F-doping ?

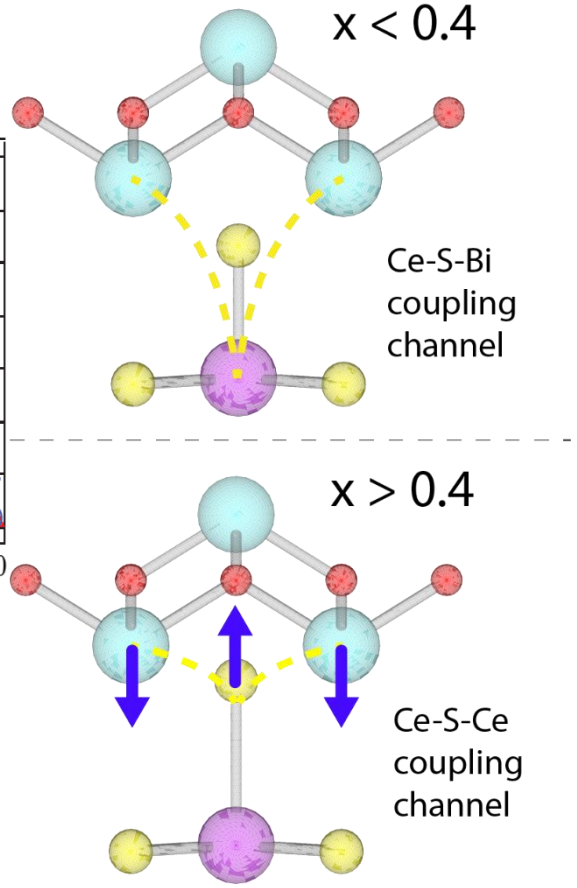
Ce L_3-edge XANES on $CeO_{1-x}F_xBiS2$

$CeO_{1-x}F_xBiS_2$ show coexistence of superconductivity and ferromagnetism when x > 0.4









Spectral weight of 4f0 decrease with F-doping and disappears for x > 0.4

Crossover from valence fluctuation to Kondo-like regime

T. Sugimoto, B. Joseph, E. Paris et al, PRB 89, 201117 (R) (2014)

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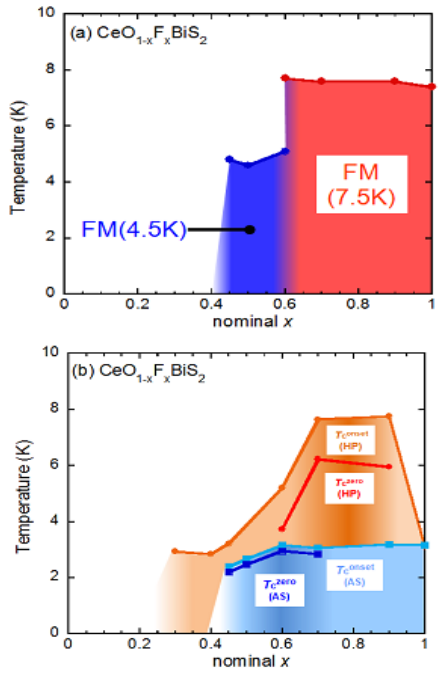

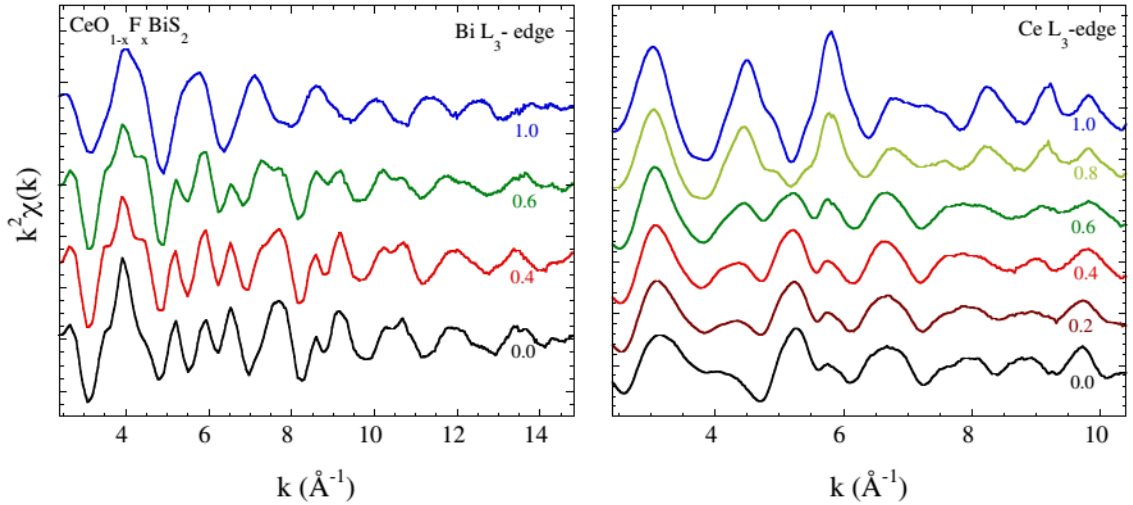

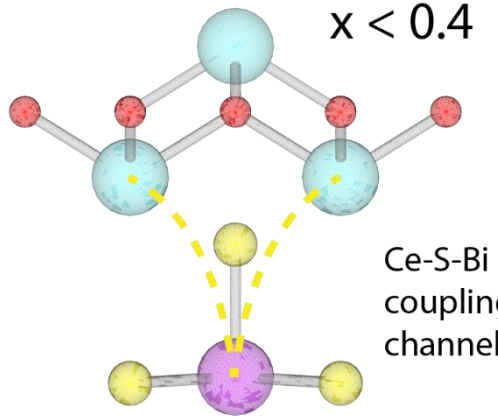

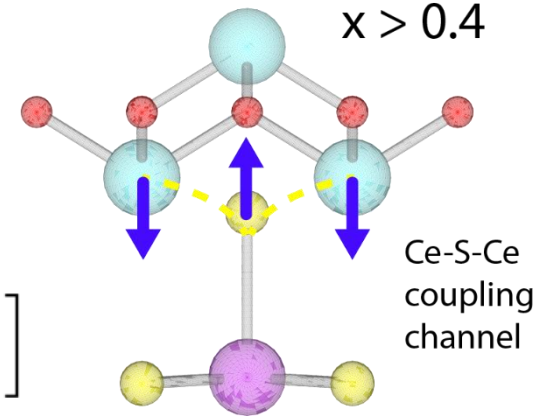

The model:

$$\chi(k) = \sum_i \frac{N_i S_0^2}{k R_i^2} f_i(k, Ri) e^{-\frac{2Ri}{\lambda}} e^{-2k^2\sigma_i^2} sin\left[2kRi + \delta_i(k)\right]$$

E. Paris et al, J. Phys. Condens. Matter 26, 435701 (2014)

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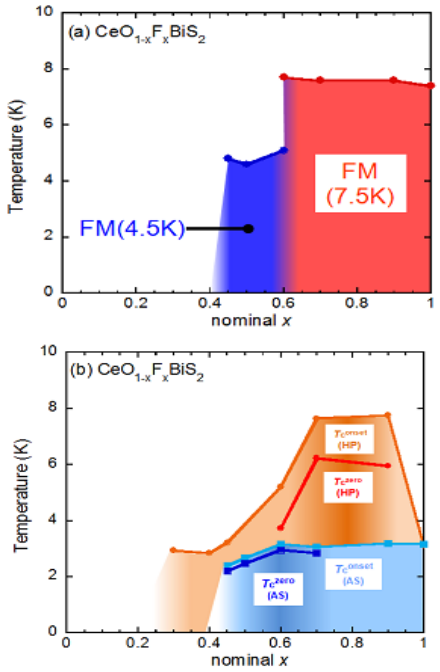
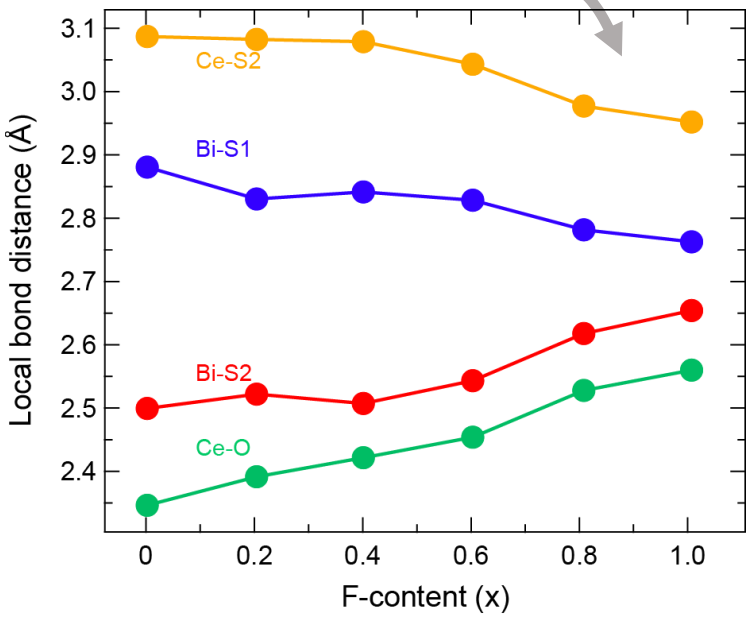
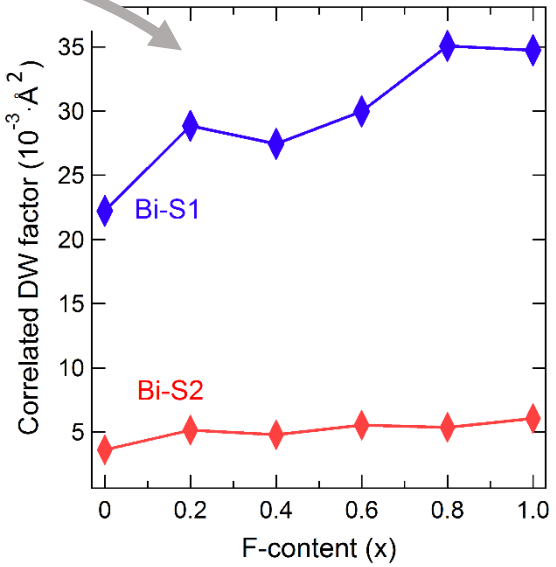
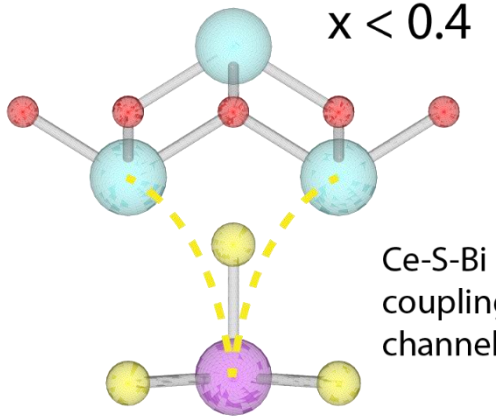
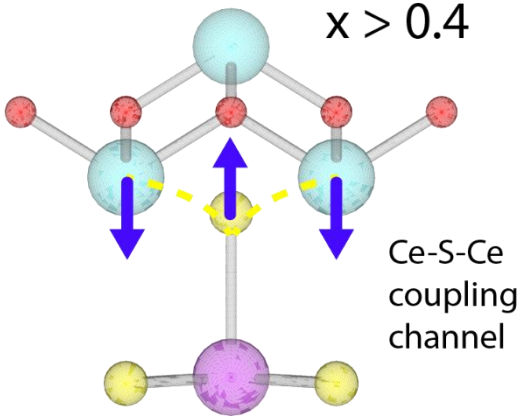


Model fit results









Interlayer coupling/decoupling is the key of the coexistence of FM and SC

E. Paris et al, J. Phys. Condens. Matter 26, 435701 (2014)

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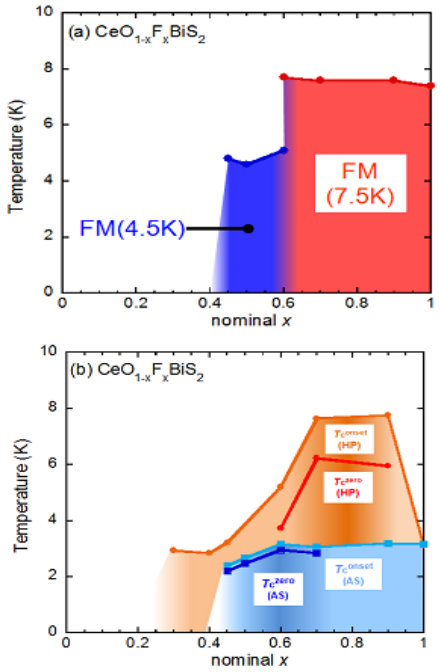

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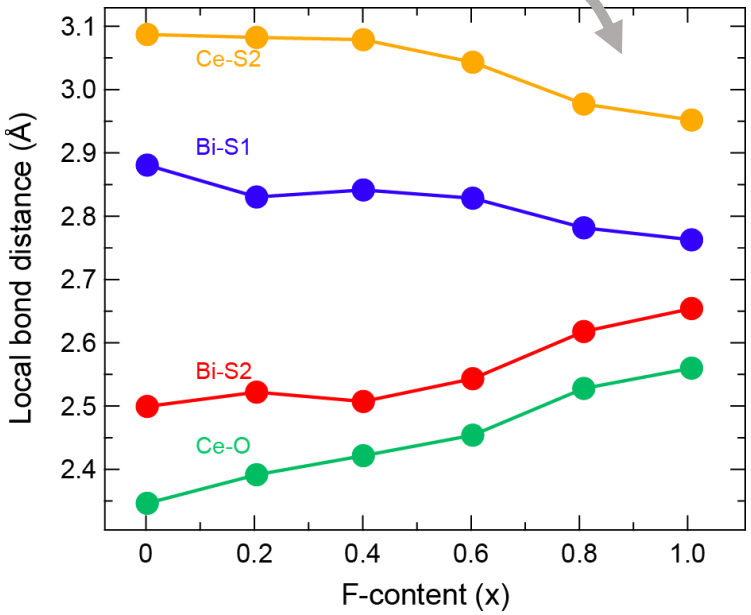
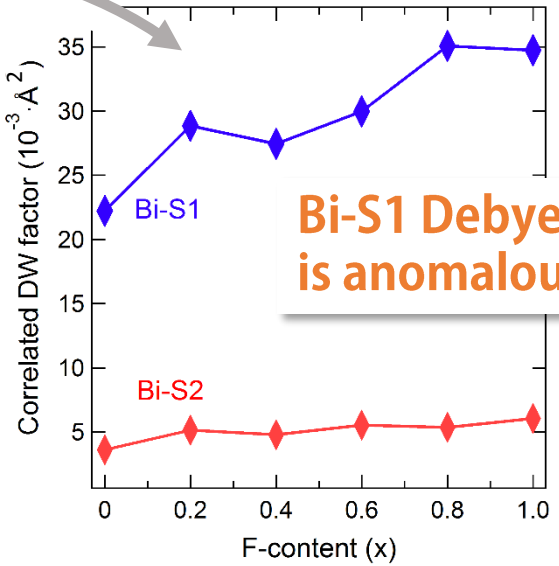
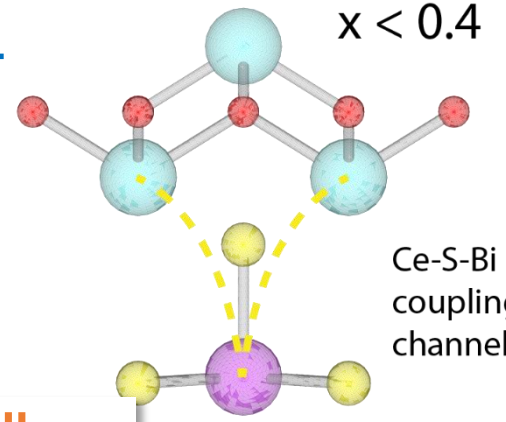
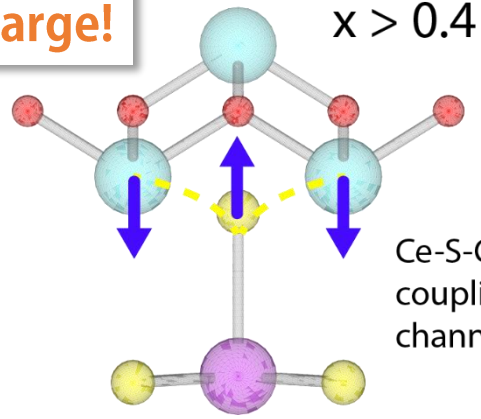




Bi-S1 Debye-Waller is anomalously large!





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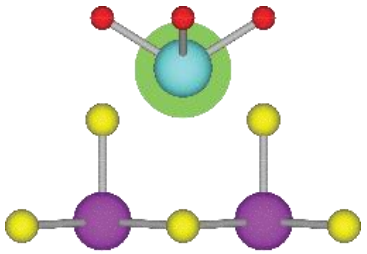
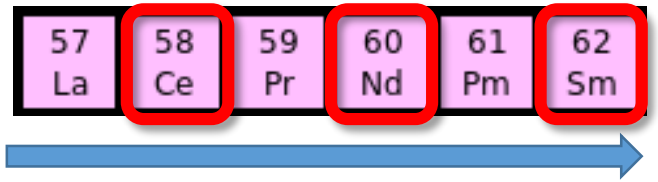
E. Paris et al, J. Phys. Condens. Matter 26, 435701 (2014)

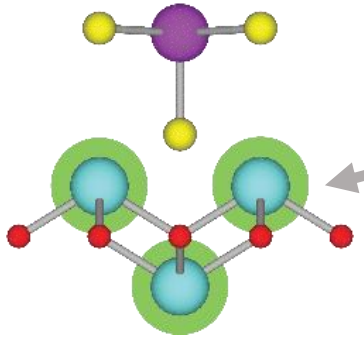
Local effect of chemical pressure ?

Bi L_3-edge EXAFS on RE(O/F)BiS_2

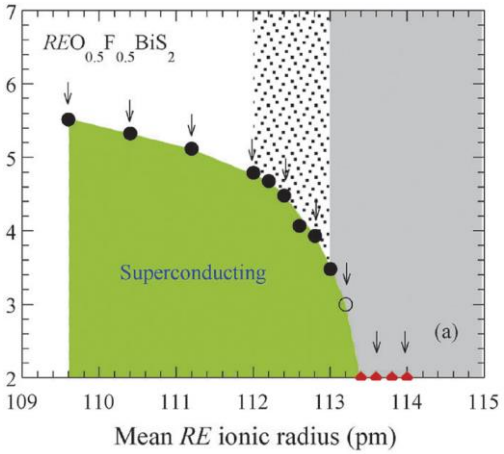
Mixing two kinds of RE^{3+} ions in the spacer layer

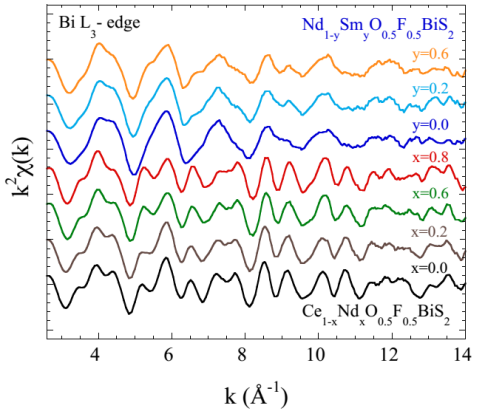


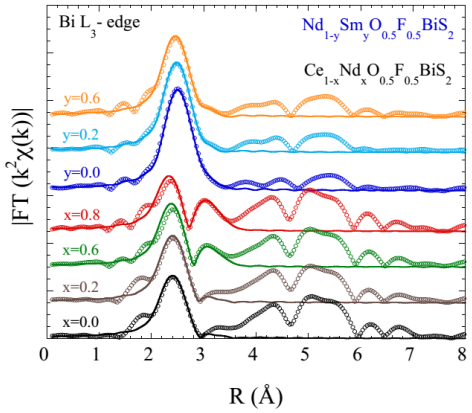




Chemical pressure!







Y. Mizuguchi, E. Paris et al, Phys. Chem Chem. Phys. 17, 22090 (2015)

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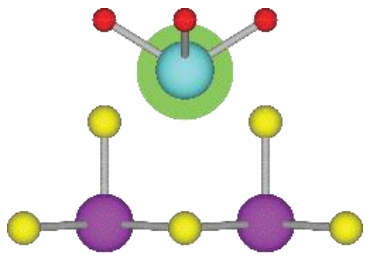
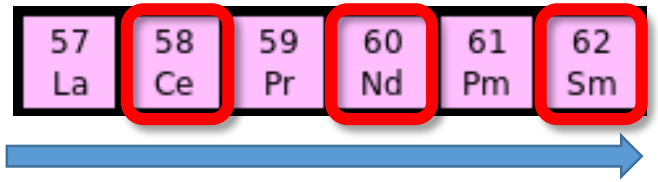
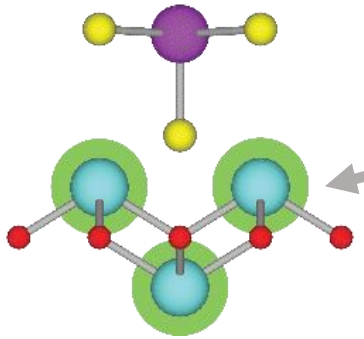
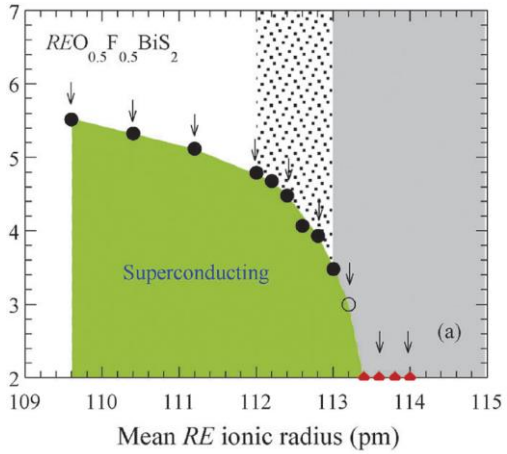
Mixing two kinds of RE^{3+} ions in the spacer layer

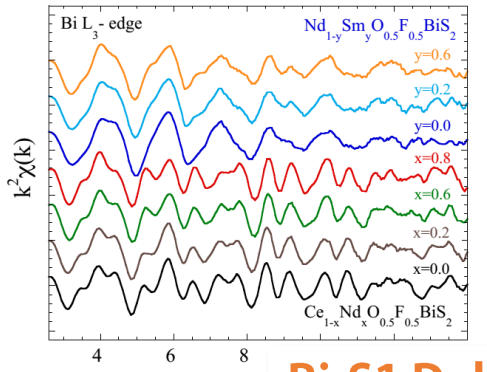


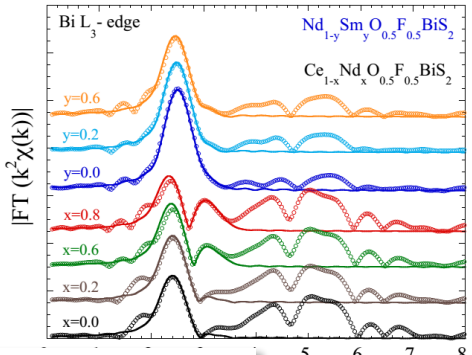




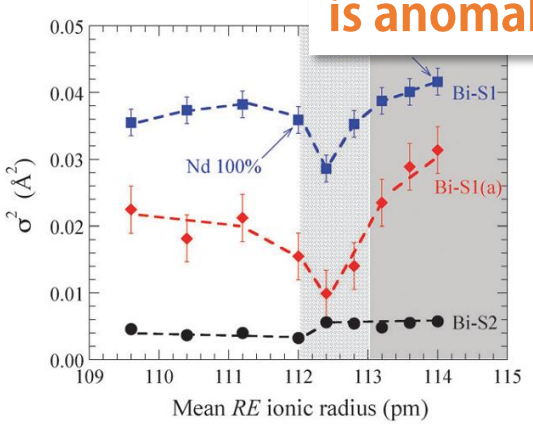
Chemical pressure!

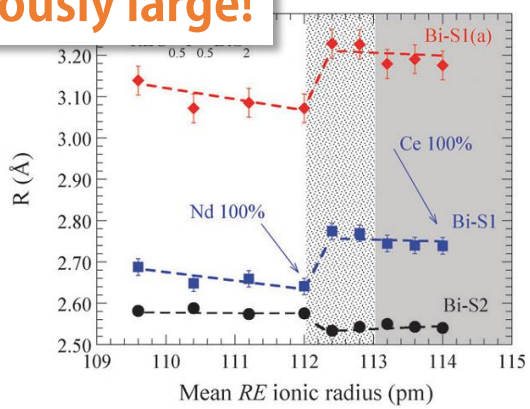






Bi-S1 Debye-Waller is anomalously large!





Y. Mizuguchi, E. Paris et al, Phys. Chem Chem. Phys. 17, 22090 (2015)

Conclusions: Local structure/function in BiS_2-materials

F-doping

- Local structure in the active layer show big evolution by doping in the spacer layer
- Correlated Debye-Waller factor for in-plane Bi-S1 bond is anomalously large
- In $CeO_{1-x}F_xBiS_2$ we provided an explanation of SC/FM coexistence in terms of local correlations

RE substitution

- From XRD and EXAFS we found clear correlation between lattice structure and superconductivity
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Meaning of the huge Bi-S1 σ^2? The in-plane Bi-S bond is highly unstable as predicted by theory

? Distortions due to chemistry of Bi 6s lone pair

? Ian-Teller like instability in Bi 6px/6py orbitals

Thank you for your attention!

What is left? ... Perspectives

F-doping How to separate disorder/local structural evolution?

Self-doped $EuFBiS_2$ system

RE substitution Effect of chemical pressure directly in the BiS_2 layer?

$REOBiS_{2-x}Se_x$

Pressure

XAS under high pressure

Meaning of the huge σ^2?

Static configurational disorder? Local bond splitting?

In-plane polarized measurements on single crystals are required!