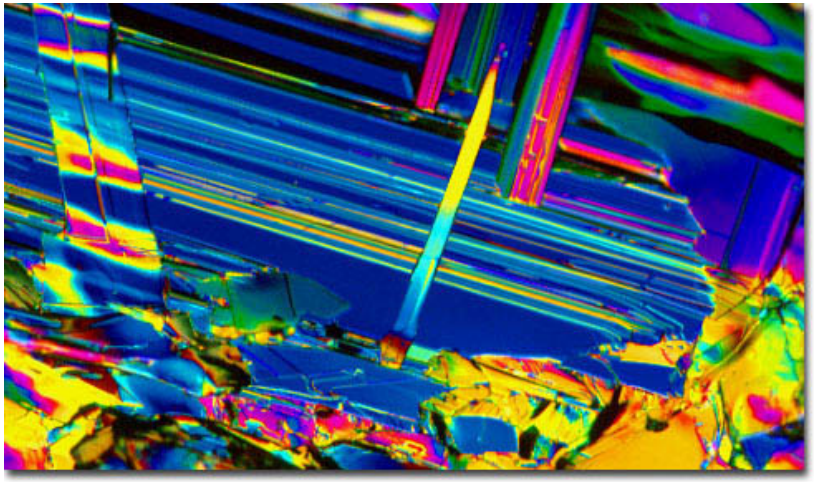
Materials Design for New Superconductors

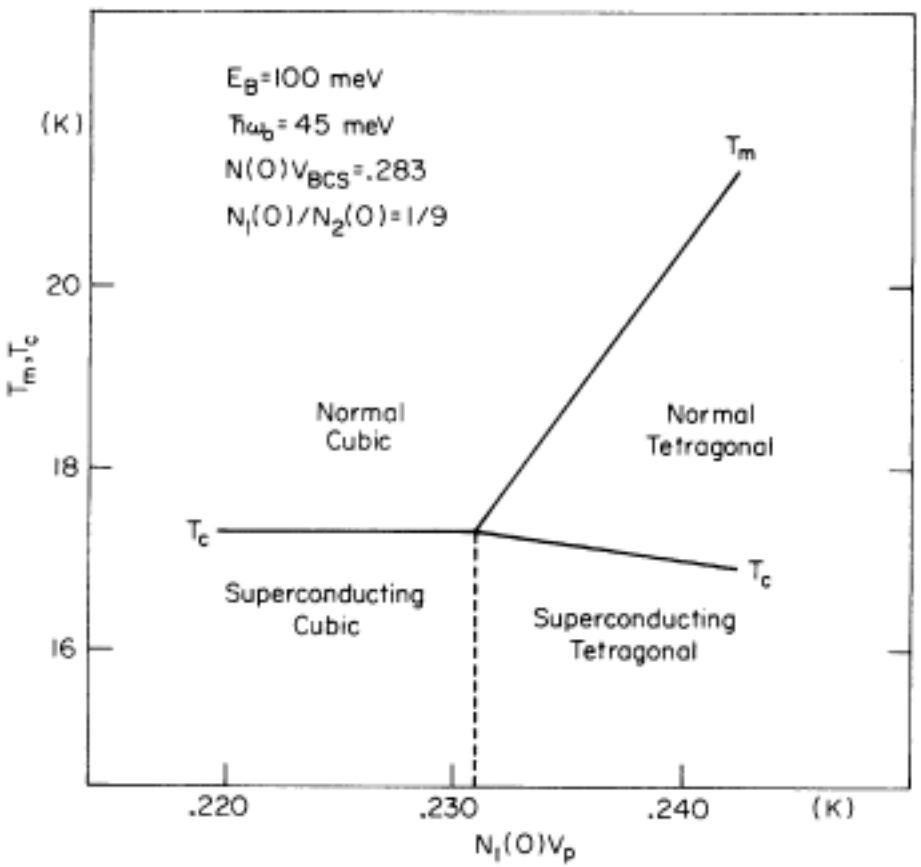
Michael Norman

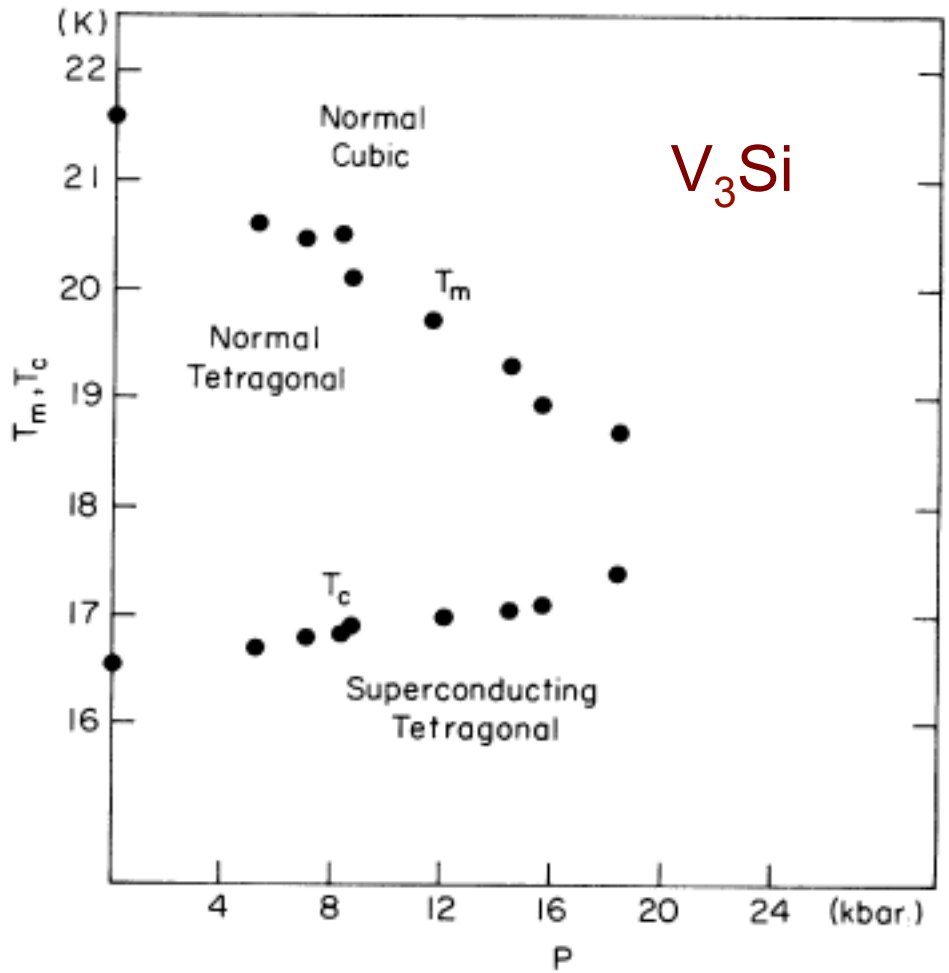
Materials Science Division
&
Center for Emergent Superconductivity
Argonne National Laboratory



UIUC – May 31, 2013

Tuning T_c near a Structural Transition

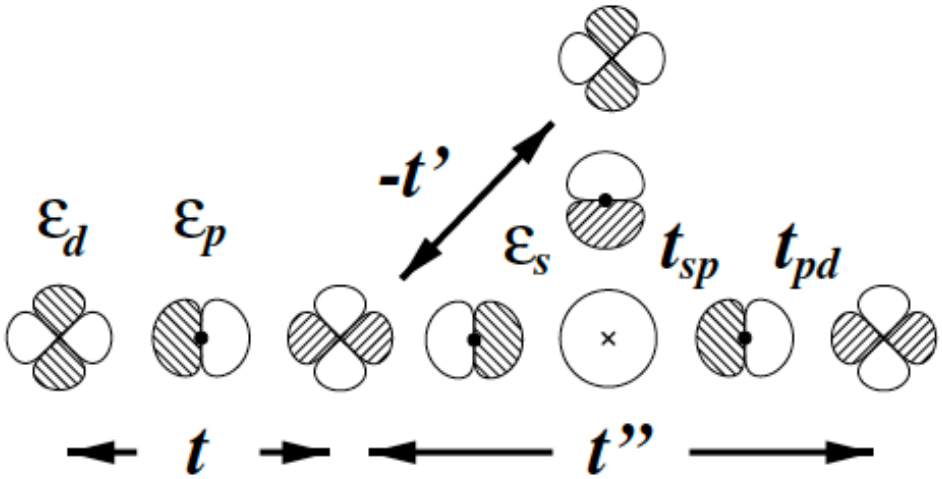


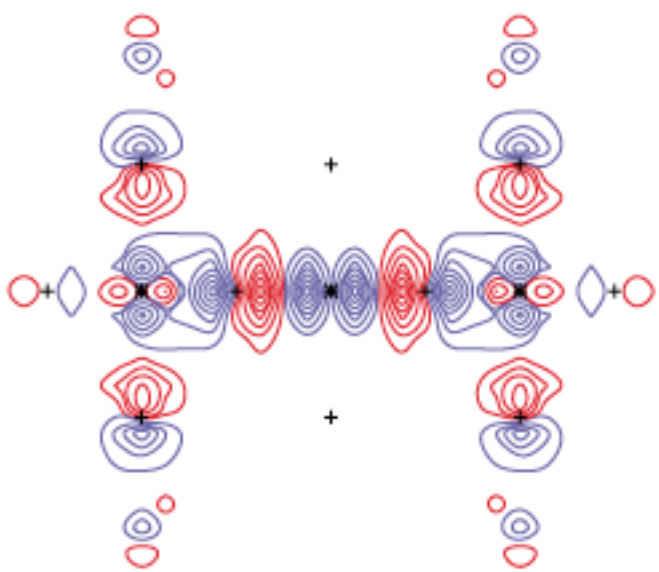


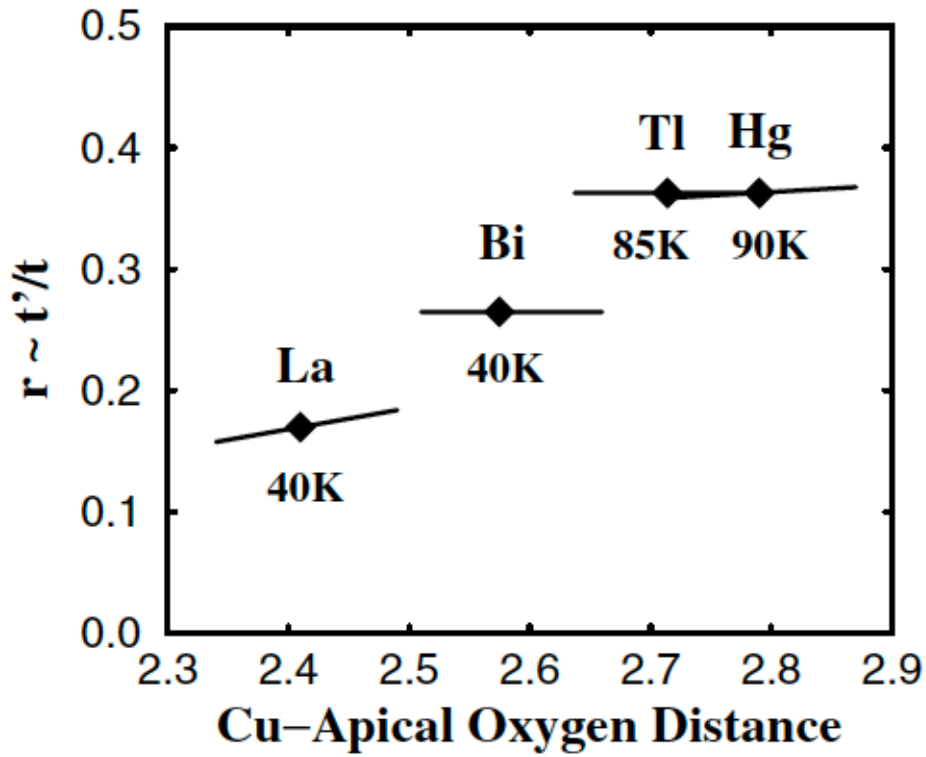
Bilbro & McMillan, PRB (1976)

Band-Structure Trend in Hole-Doped Cuprates and Correlation with $T_{c\,\max}$

E. Pavarini, I. Dasgupta,* T. Saha-Dasgupta,† O. Jepsen, and O. K. Andersen

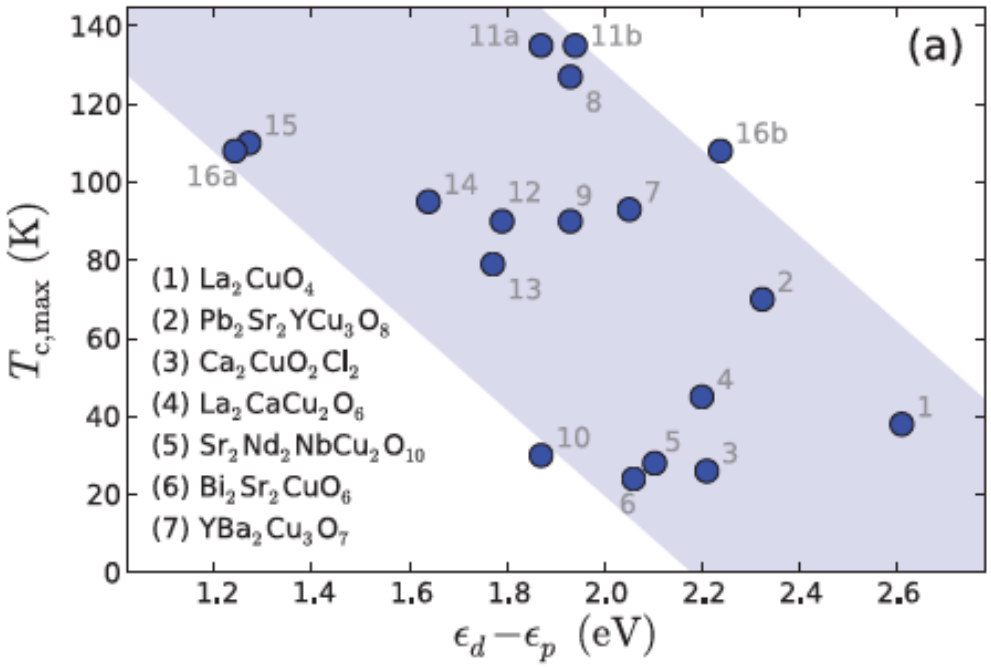


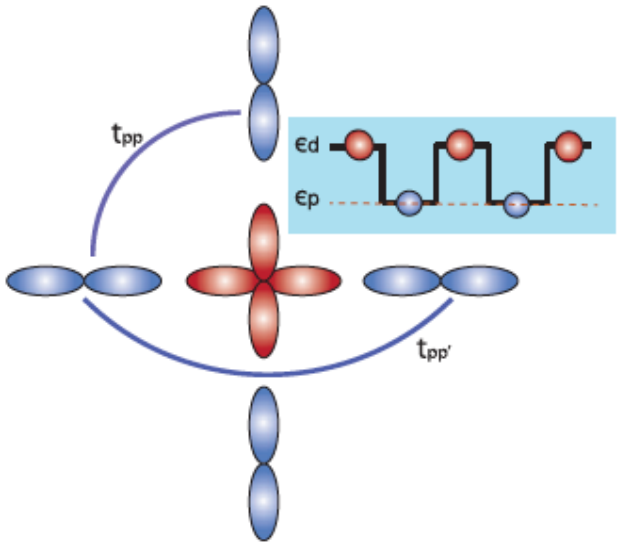


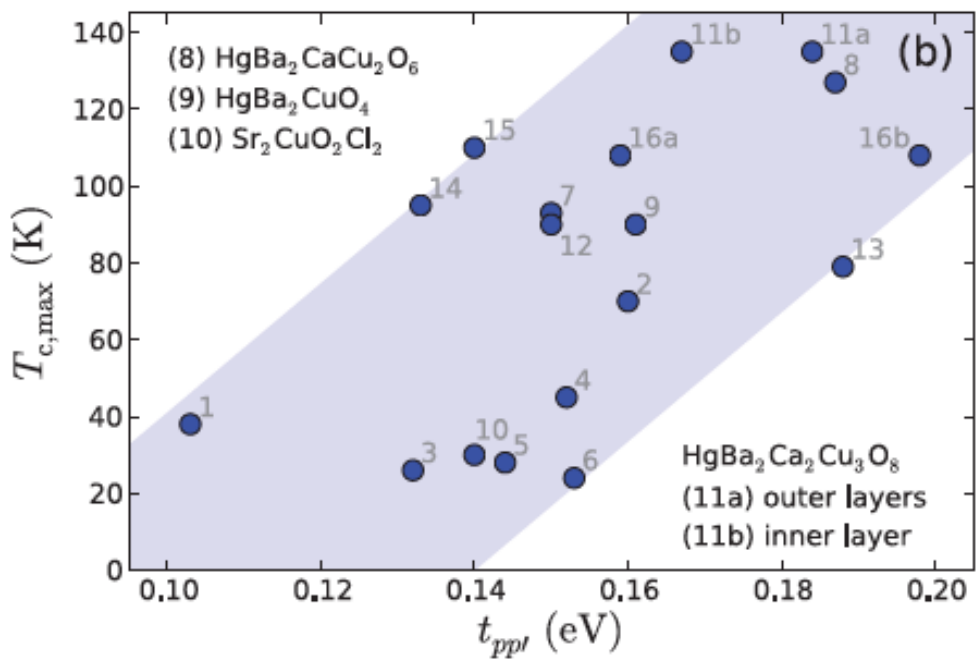


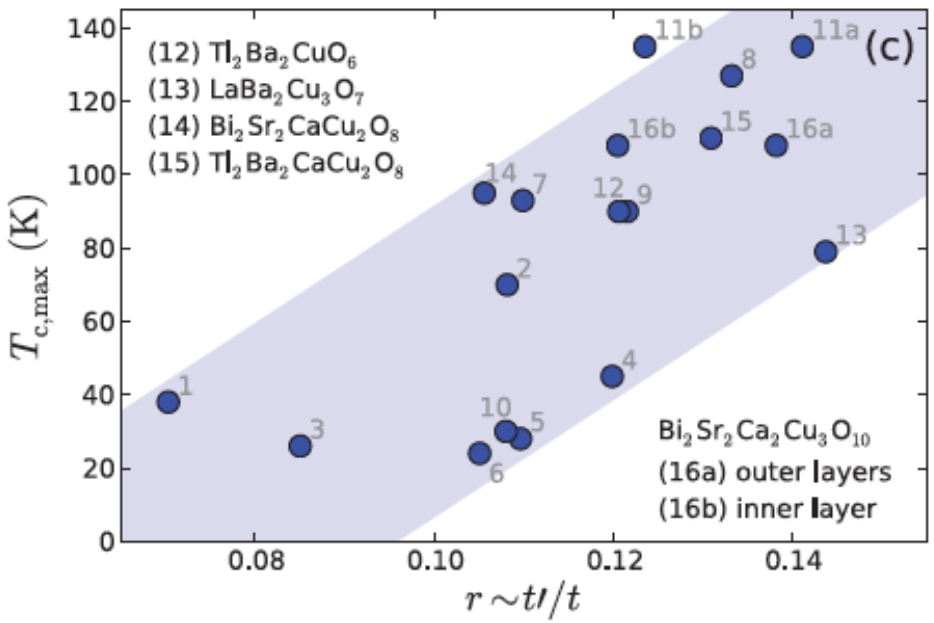
Pavarini *et al*, PRL (2001)

Cluster DMFT



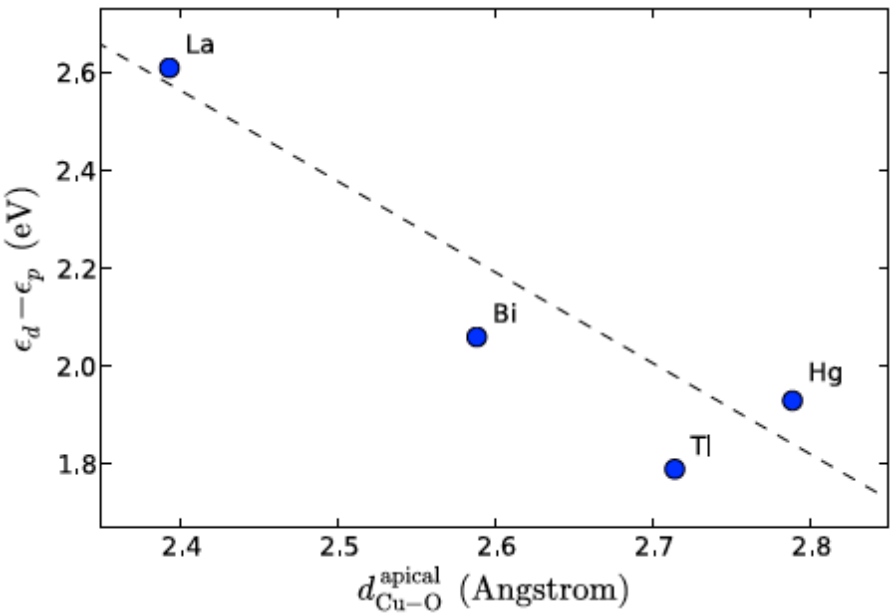


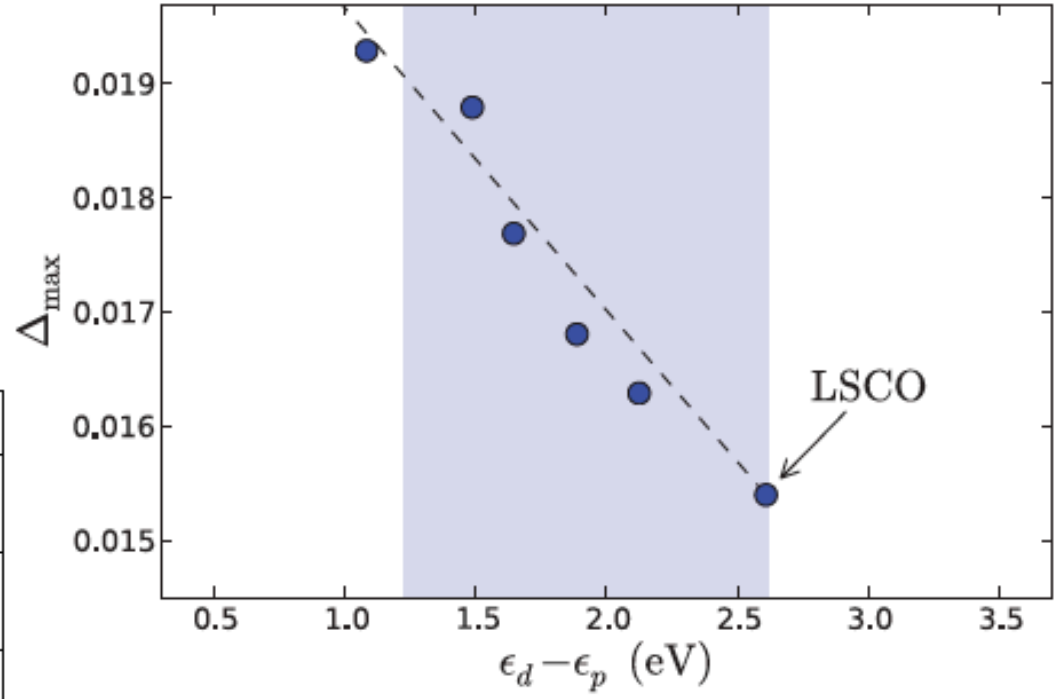


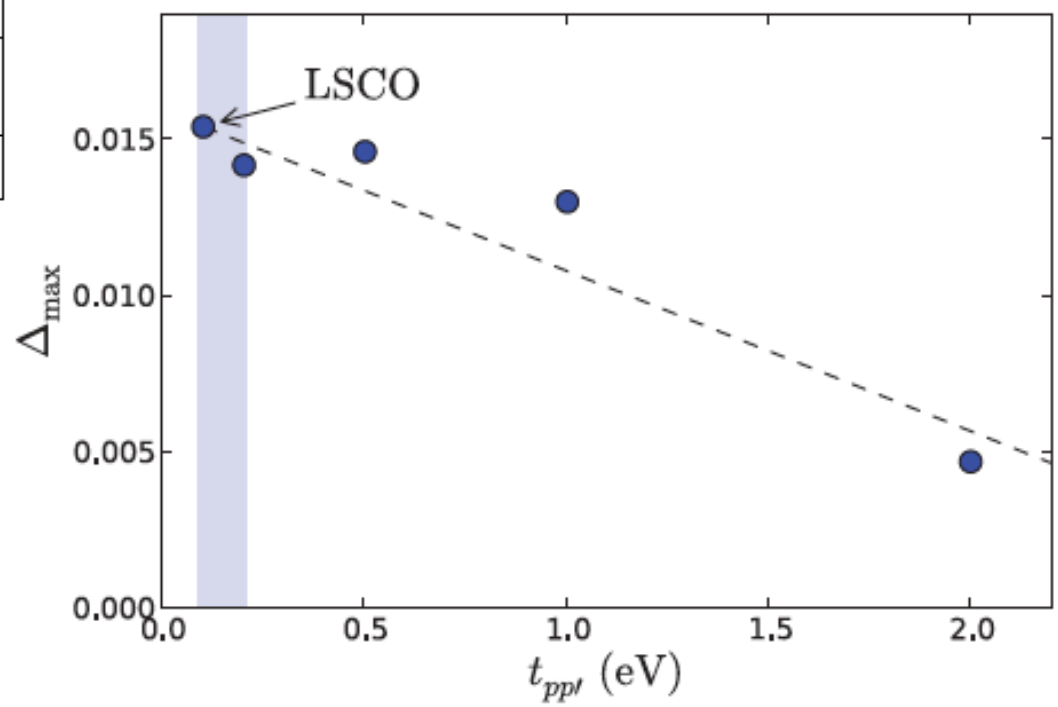


Weber *et al.*, EPL (2012)

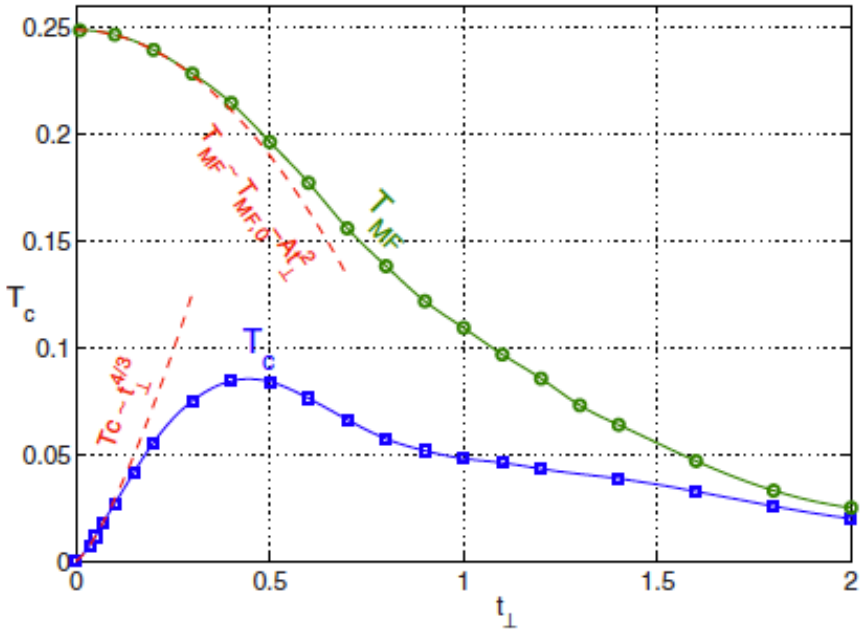
T_c vs ε_p-ε_d



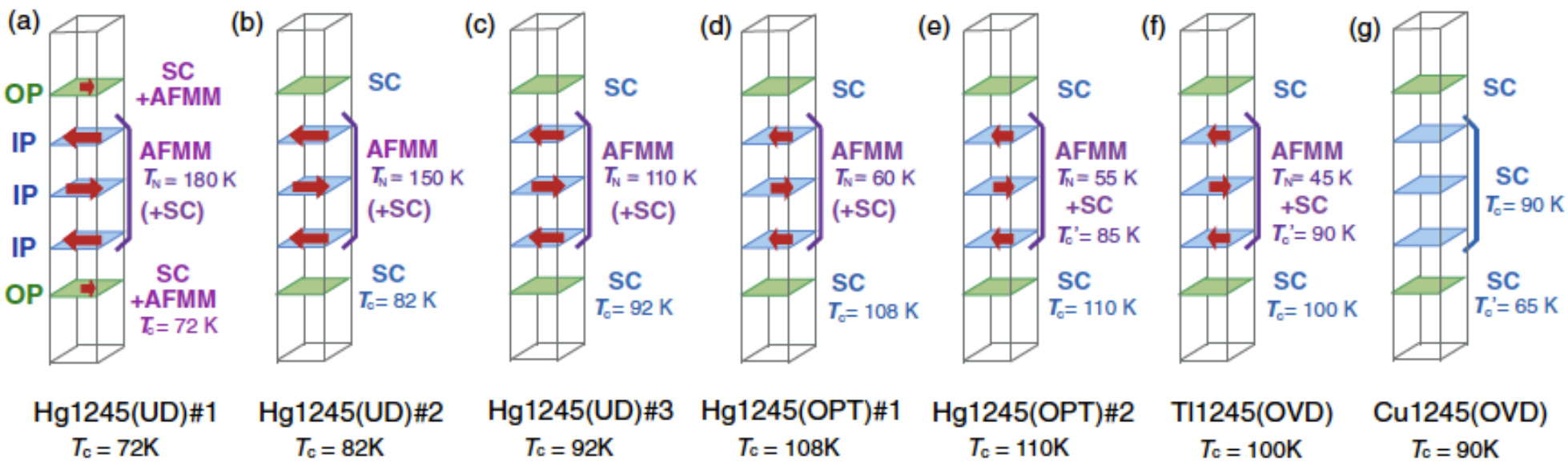




Composite Systems – A route to higher T_c

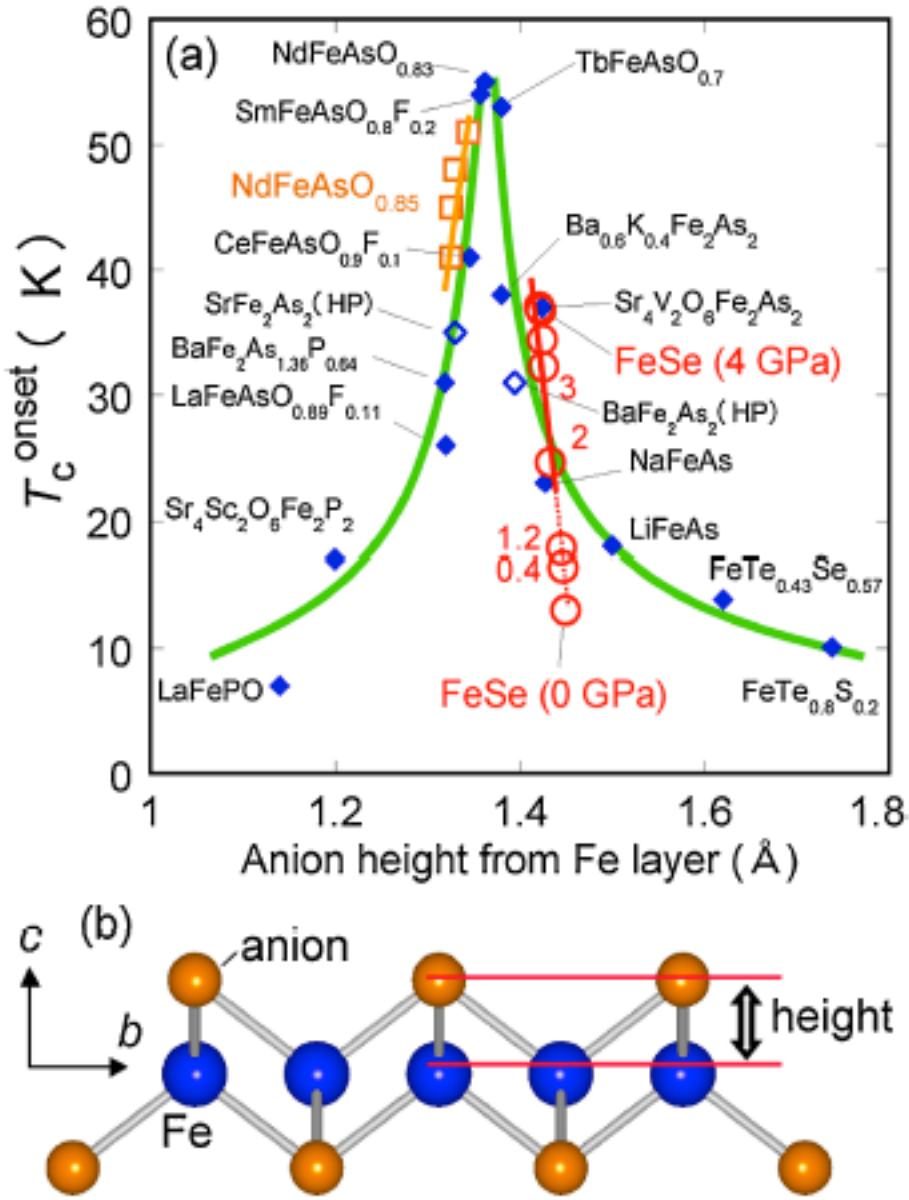


Berg *et al.*, PRB (2008)



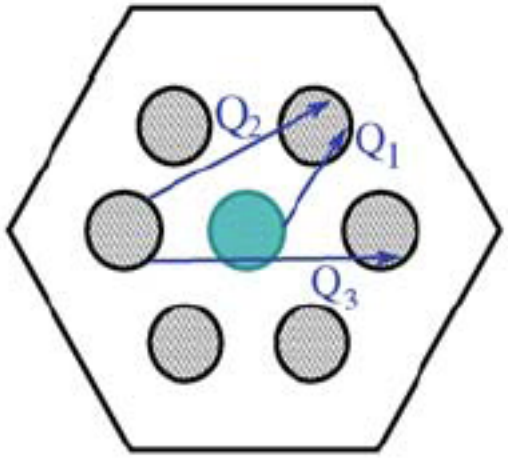
Mukuda *et al.*, JPSJ (2012)

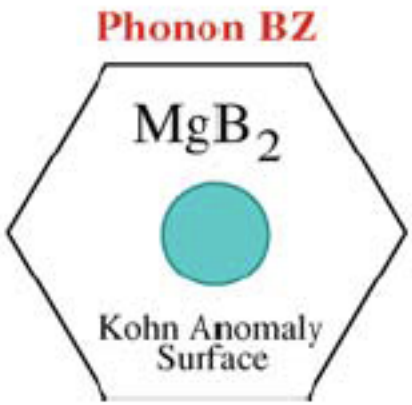
Tuning T_c in iron pnictides/chalcogenides via anion height

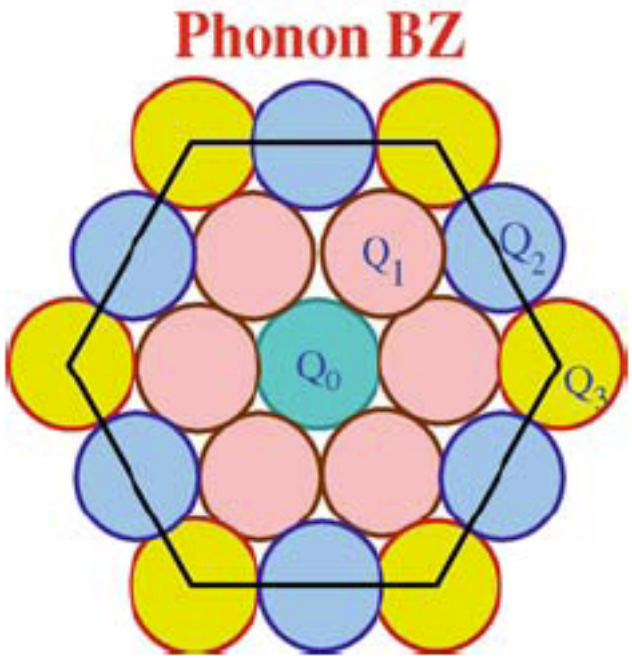


Mizuguchi & Takano, JPSJ (2010)

Filling up the Brillouin Zone

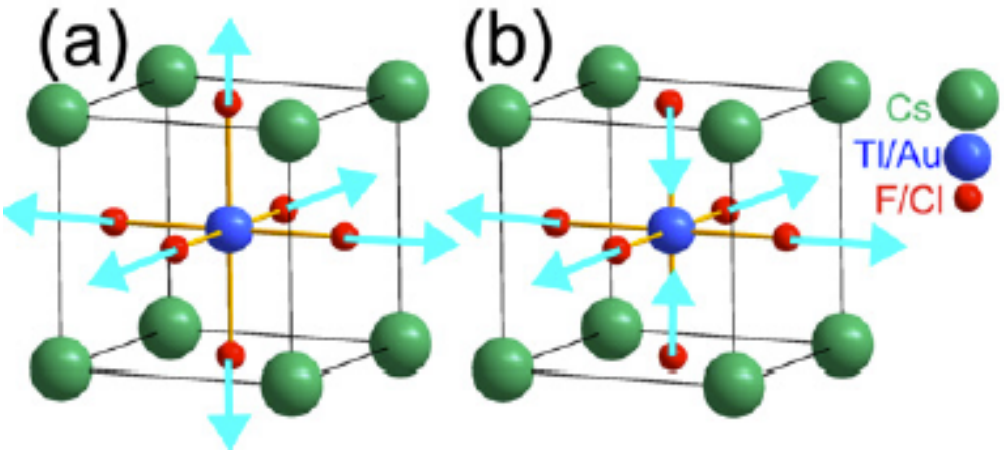


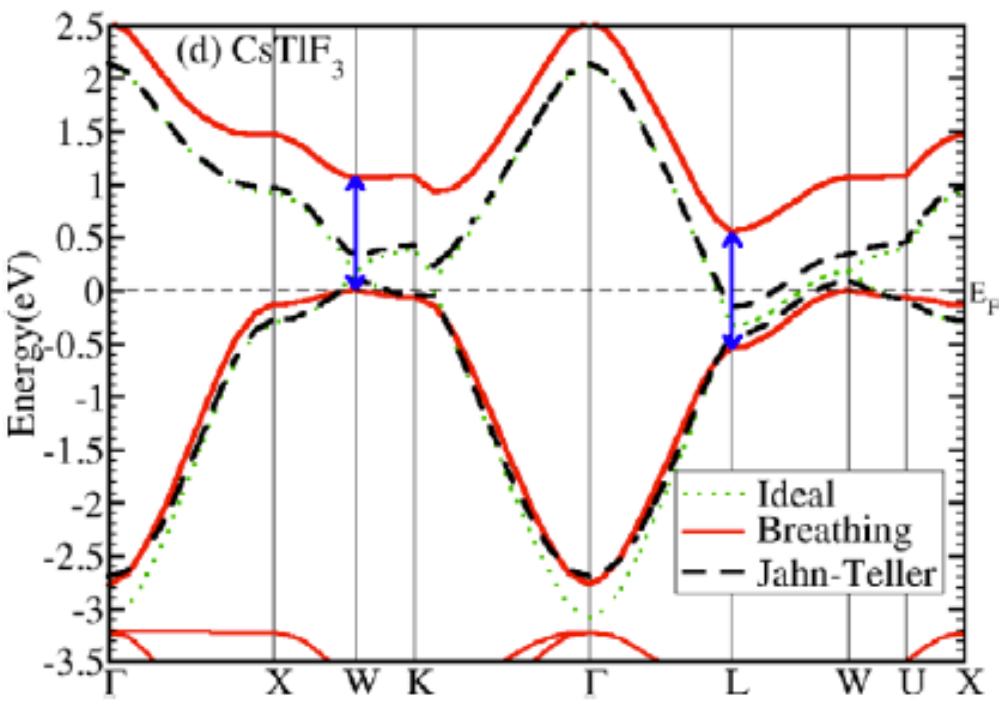


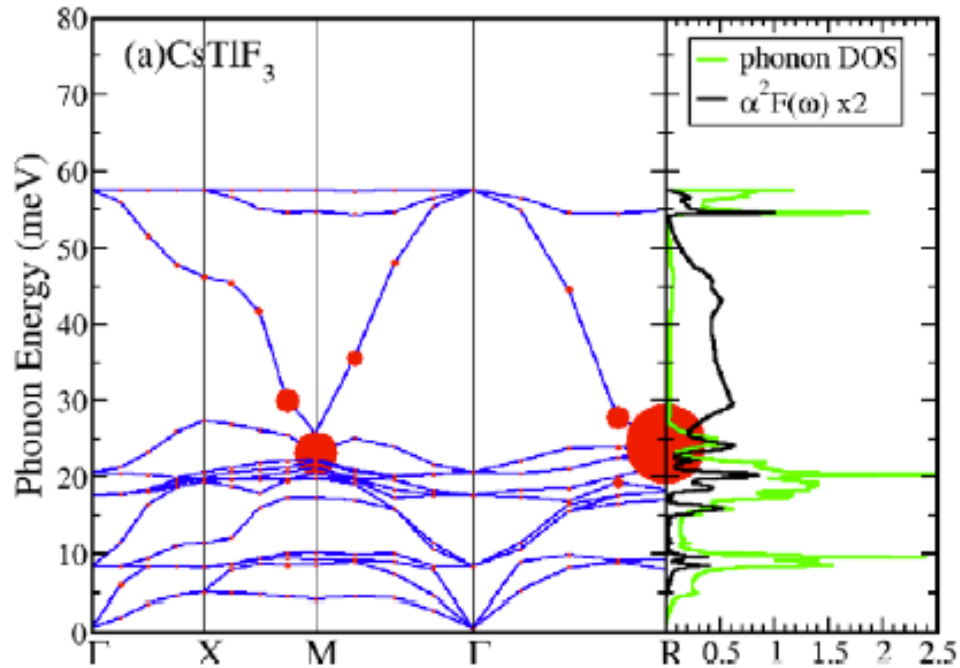


Pickett, J Superconductivity (2006)

Rational Materials Design ($CsTlF_3$ & $CsTlCl_3$)

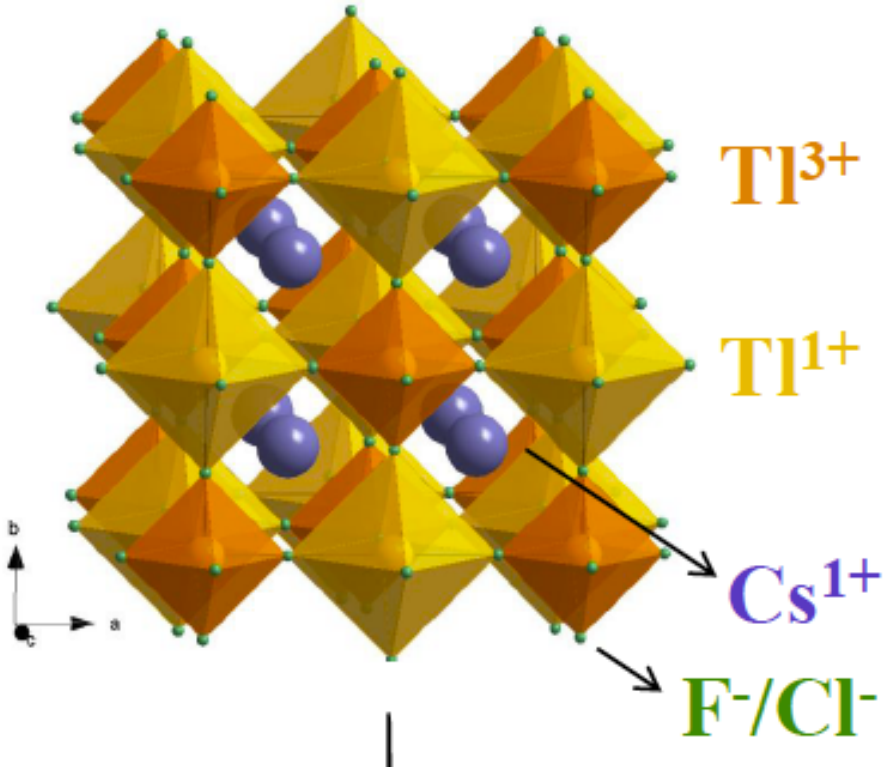


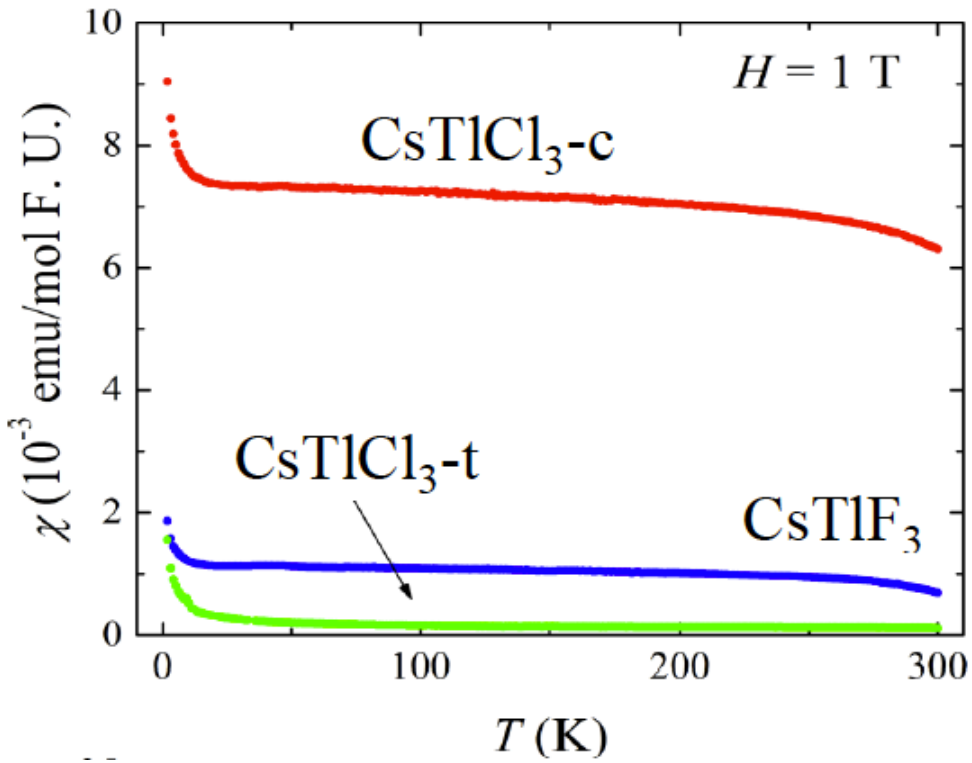




Yin & Kotliar, EPL (2013)

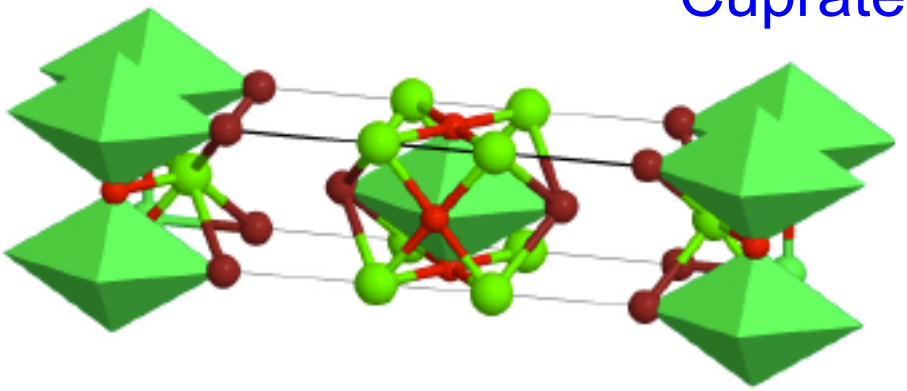
Synthesized



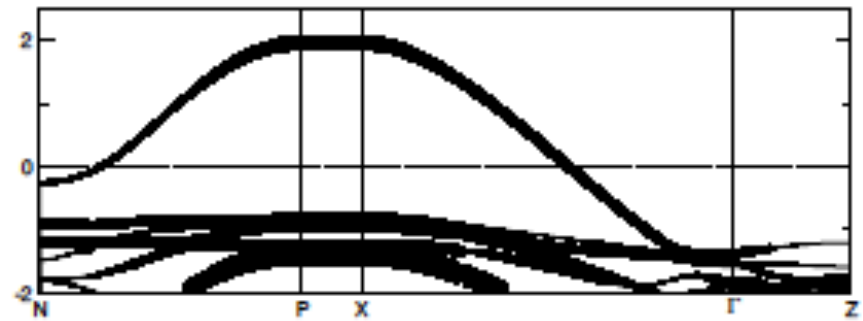


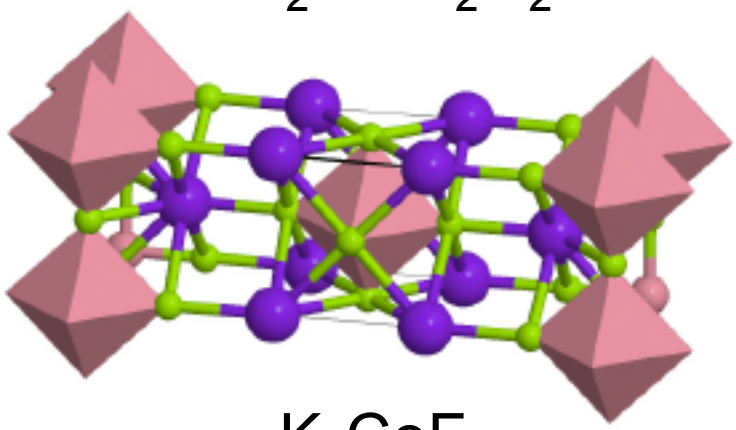
Retuerto *et al*, arXiv:1302.2353

Data Mining (over 60,000 electronic structures)
Cuprate analogues?

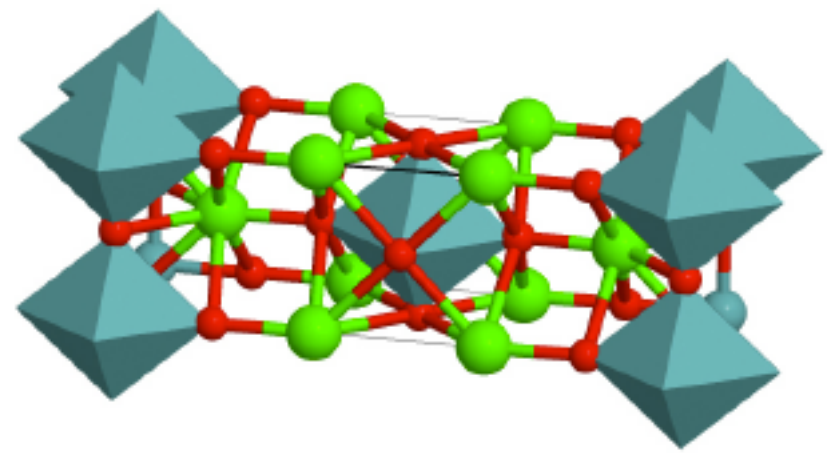


$Ca_2CuBr_2O_2$

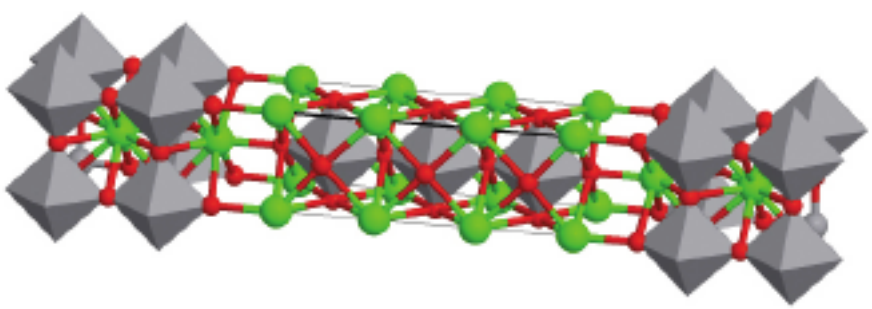




K_2CoF_4



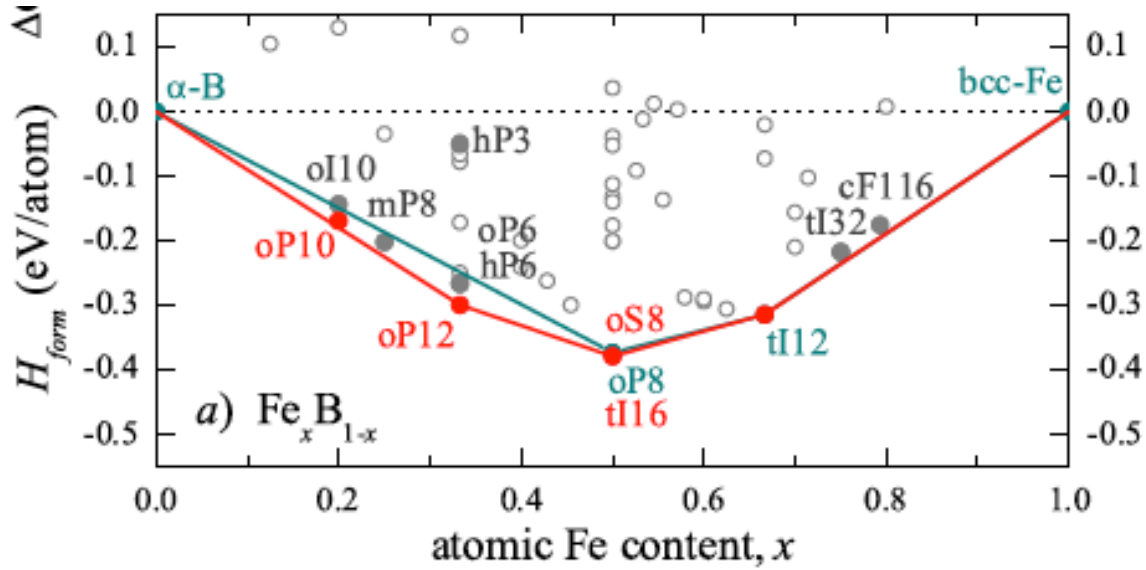
Sr_2MoO_4

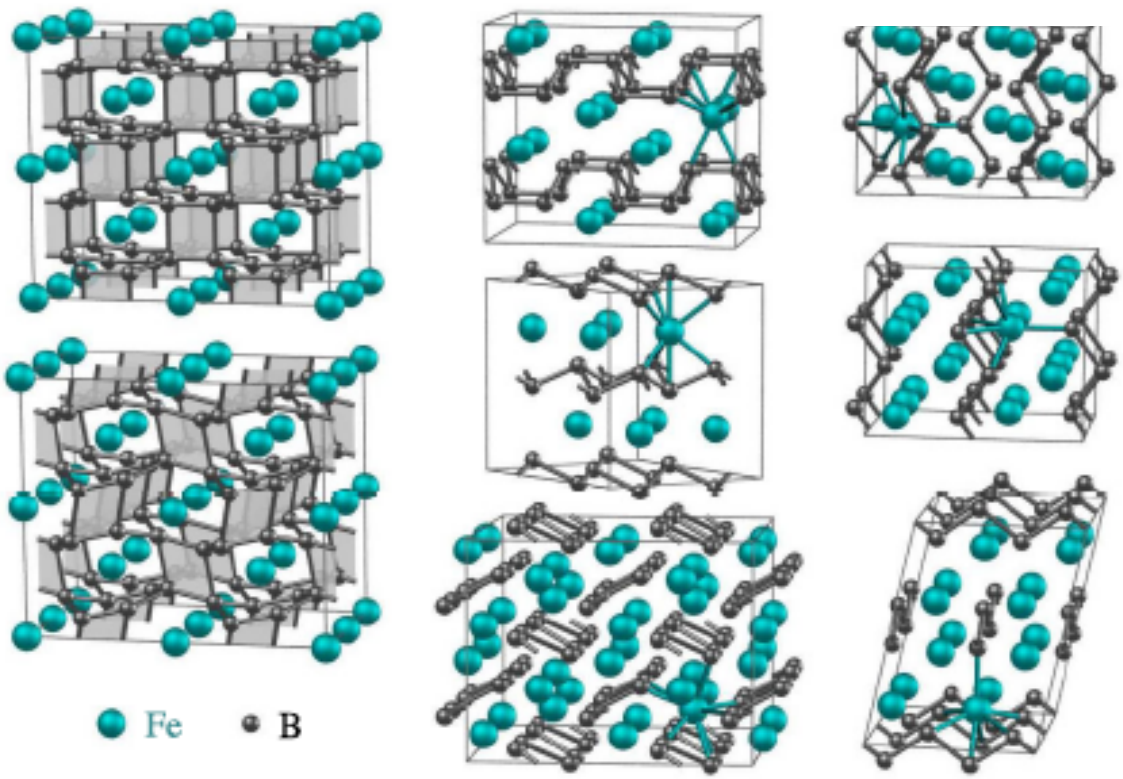


$Sr_4V_3O_{10}$

Klintenberg & Eriksson, Comp Matls Sci (2013)

Evolutionary Search - FeB





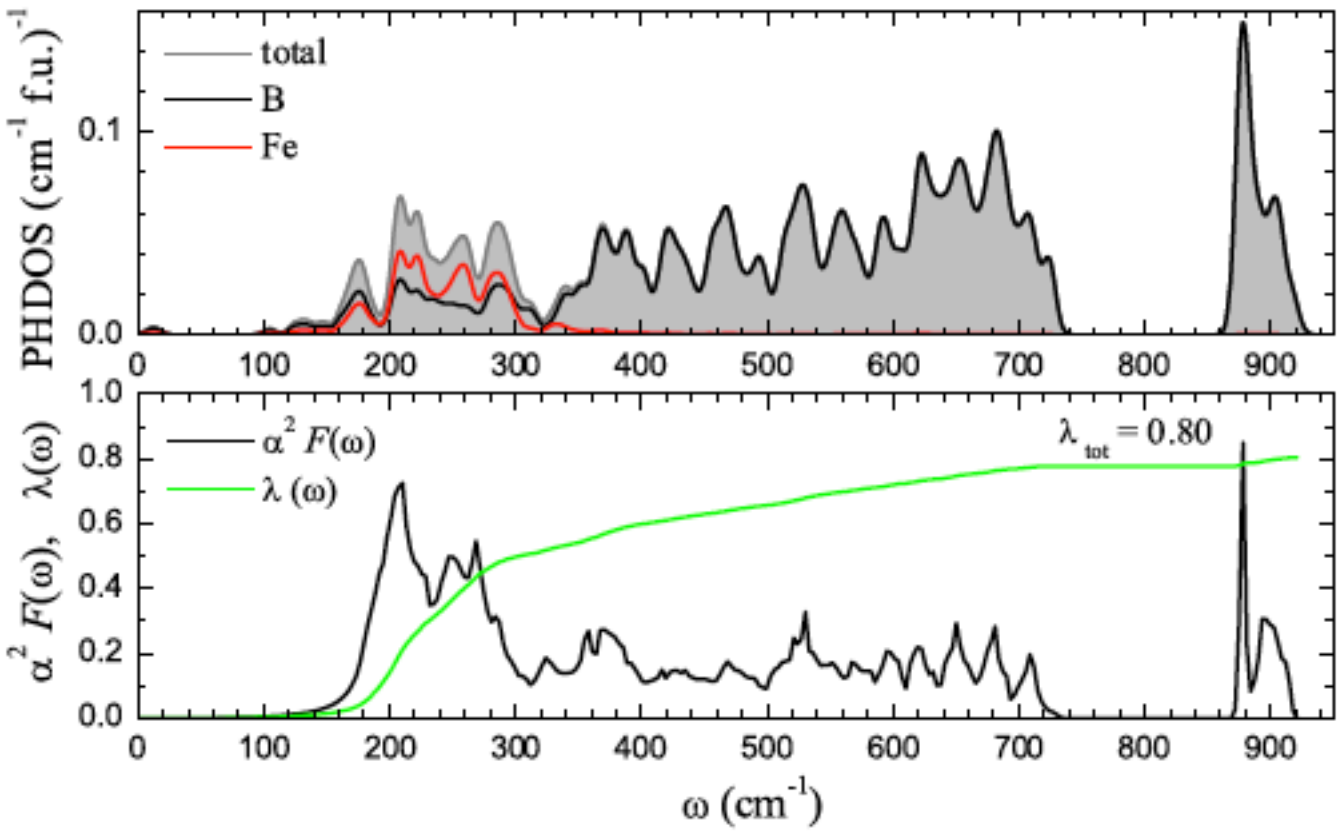
oI10-FeB_4
oP10-FeB_4 (new)

oP6-FeB_2
hP6-FeB_2
oP12-FeB_2 (new)

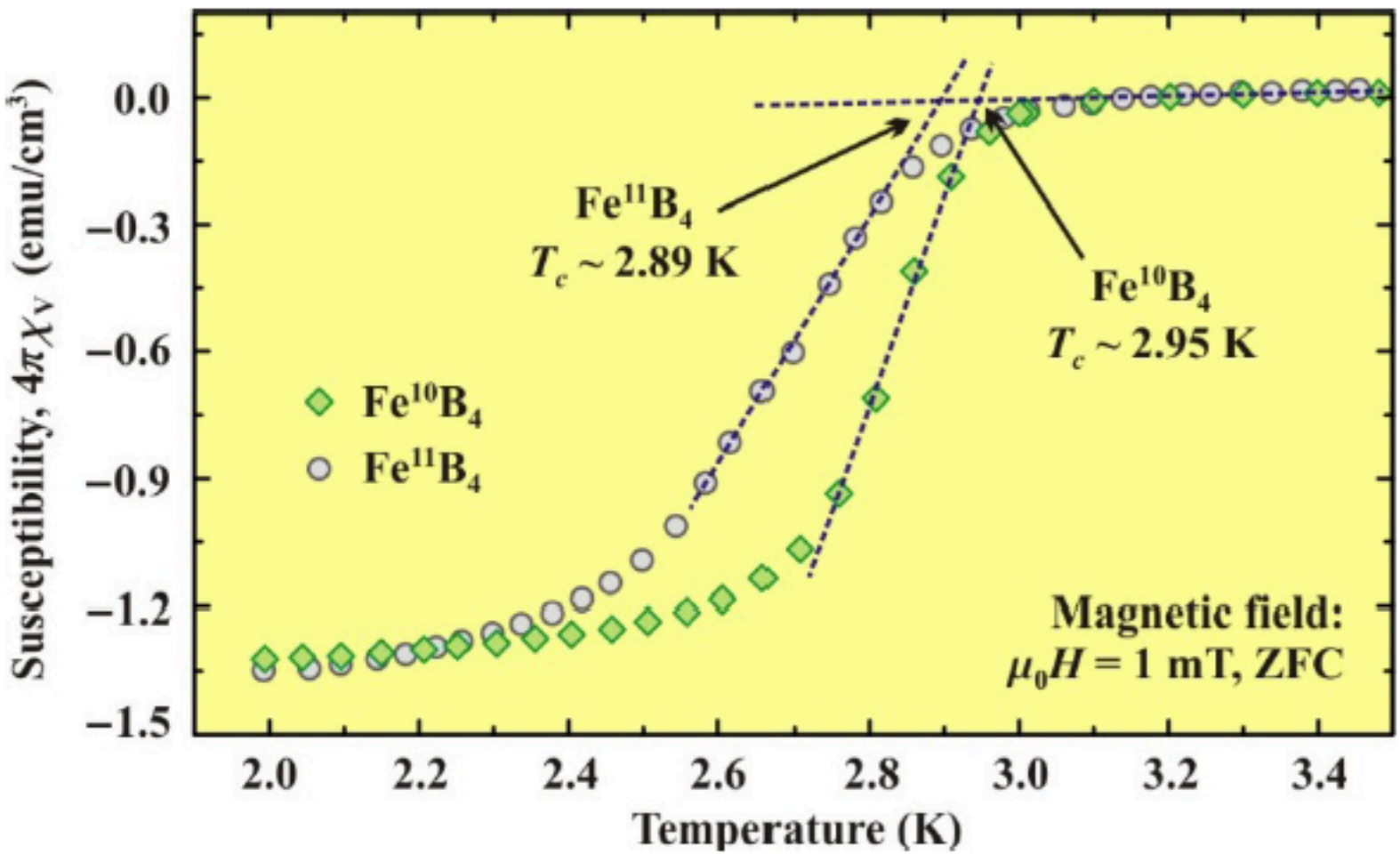
oP8-FeB
oS8-FeB
tI16-FeB

Kolmorgorov *et al*, PRL (2010)

Predicted Superconductivity in *oP*10-FeB_4

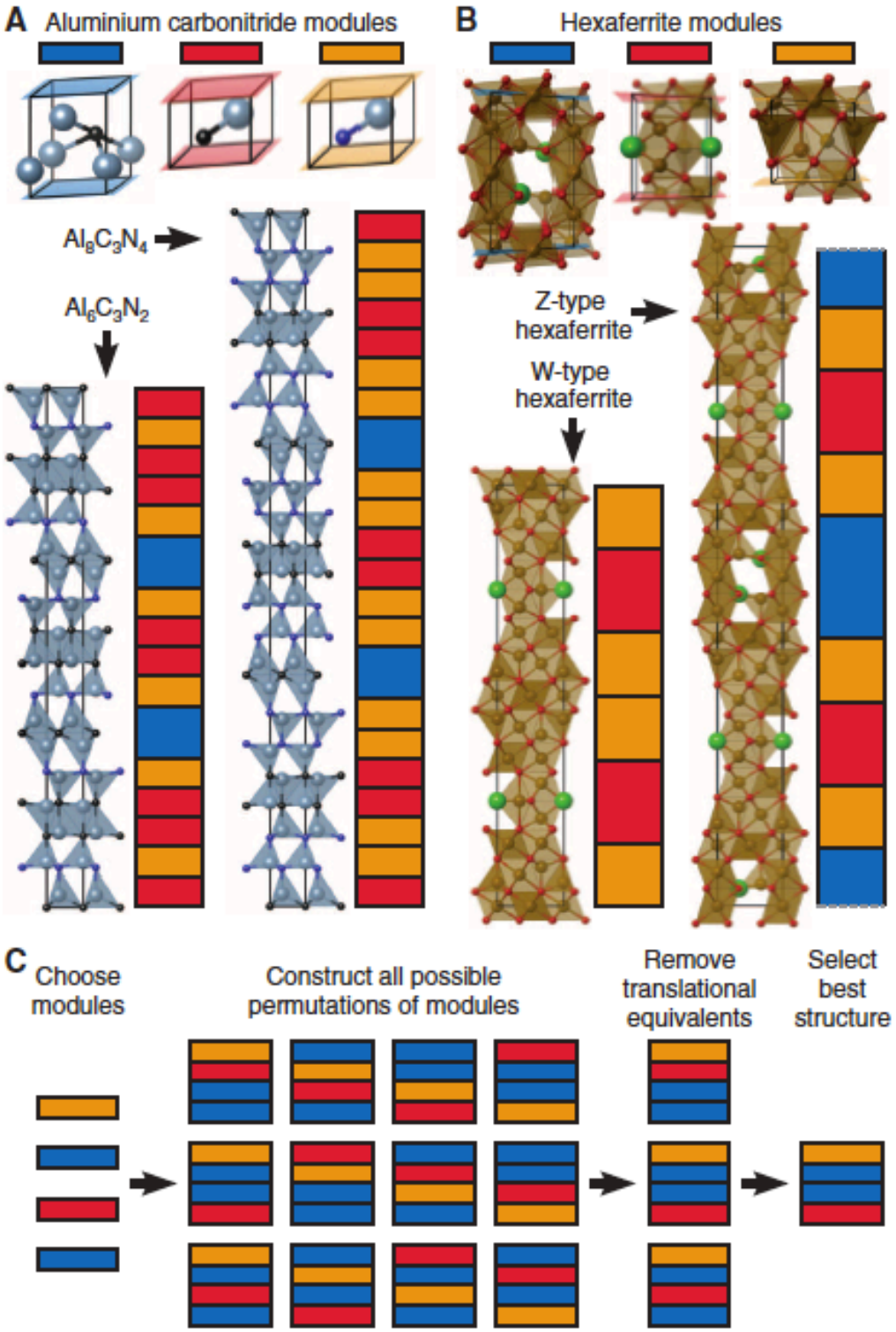


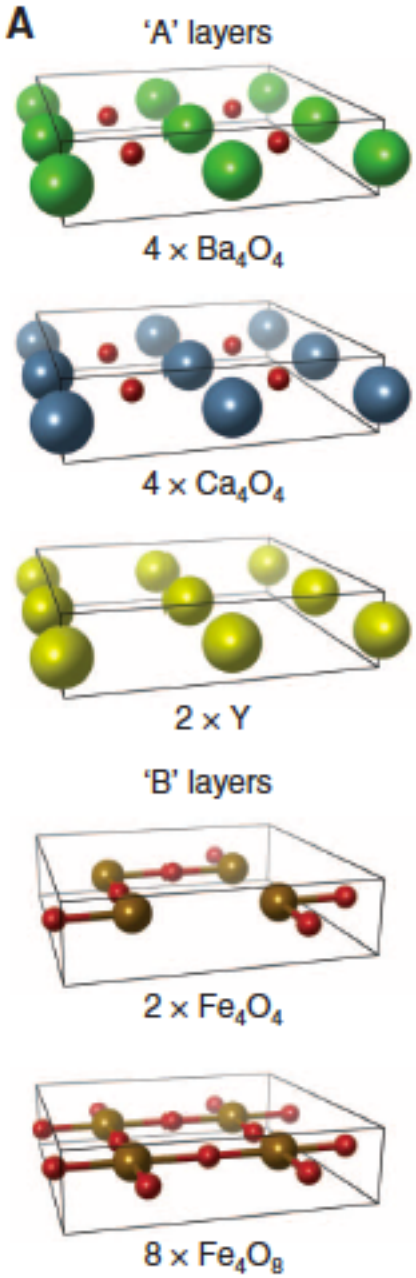
Synthesized and found to have a T_c of 3K



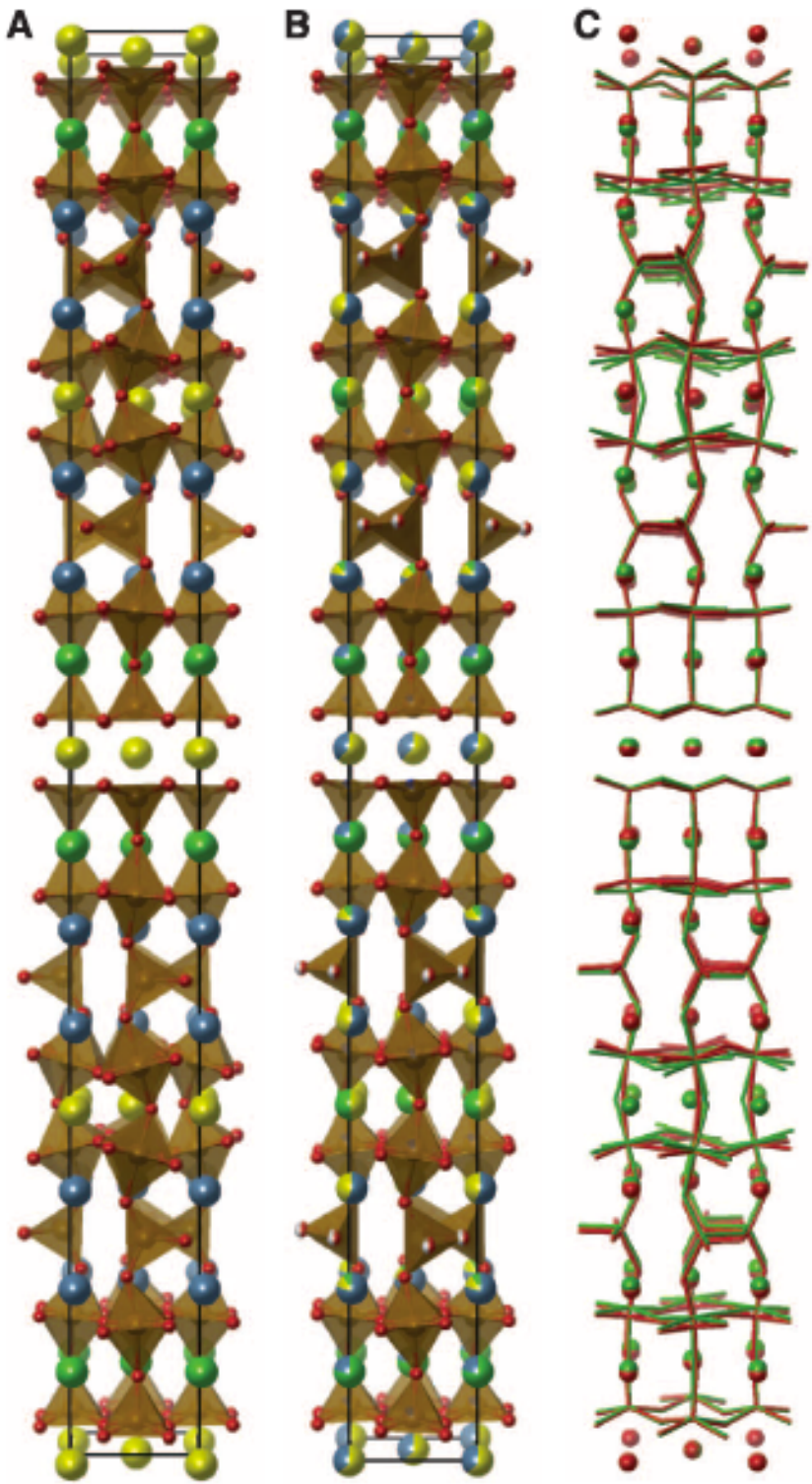
Gou *et al*, arXiv:1304.5106

Modular Construction



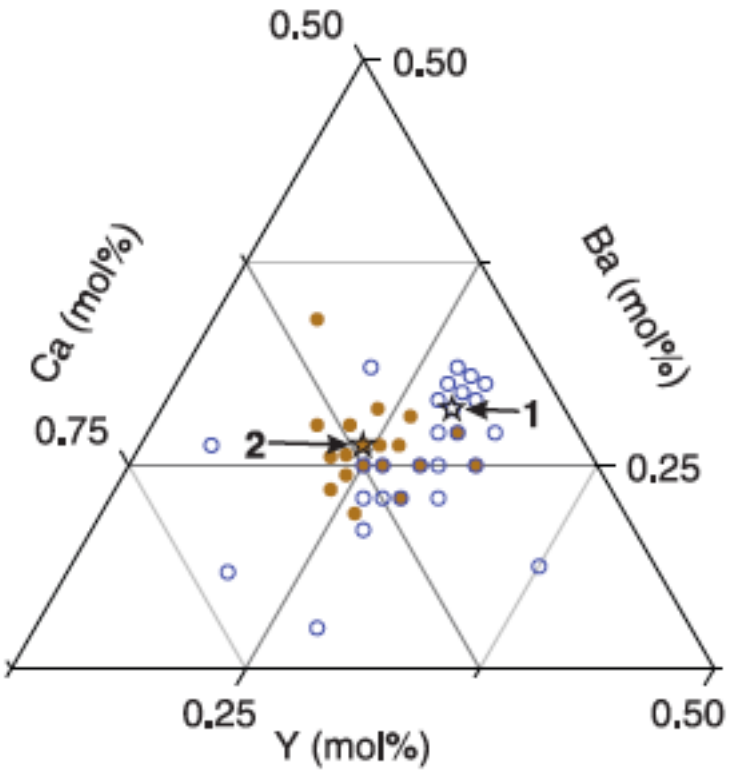


Dyer *et al*, Science (2013)

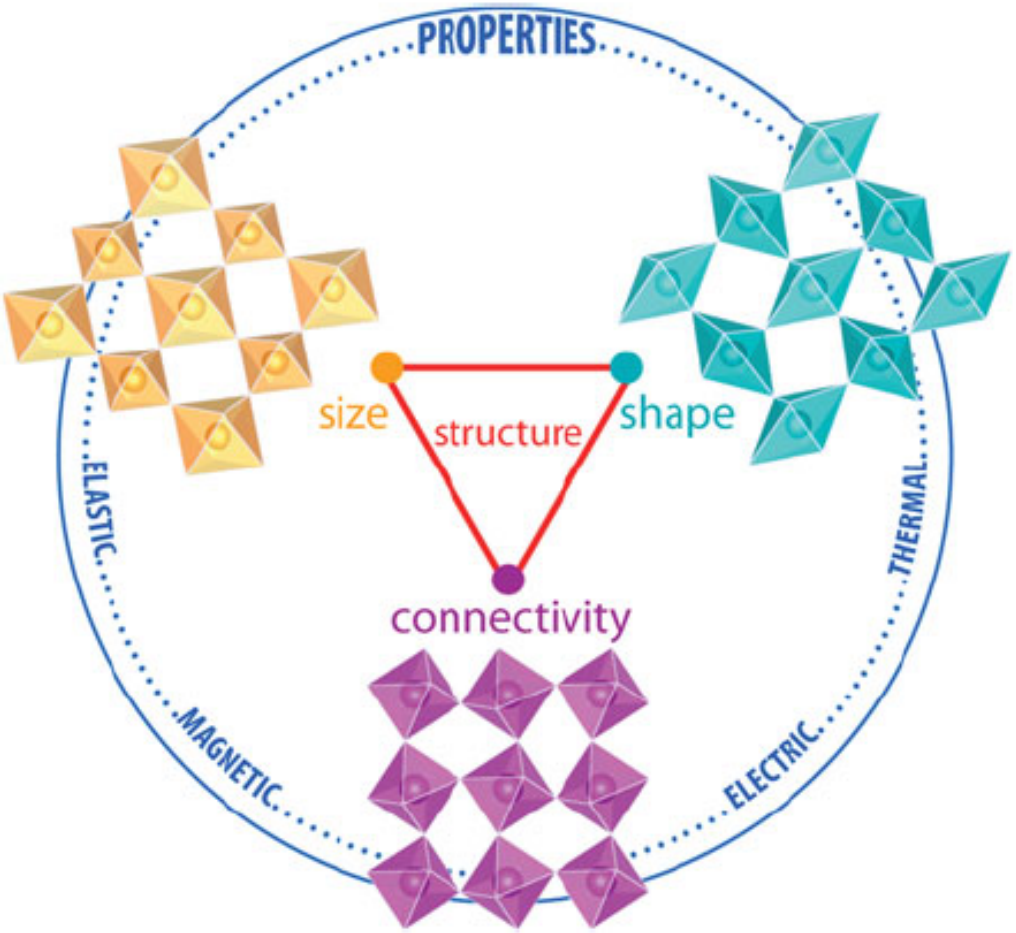


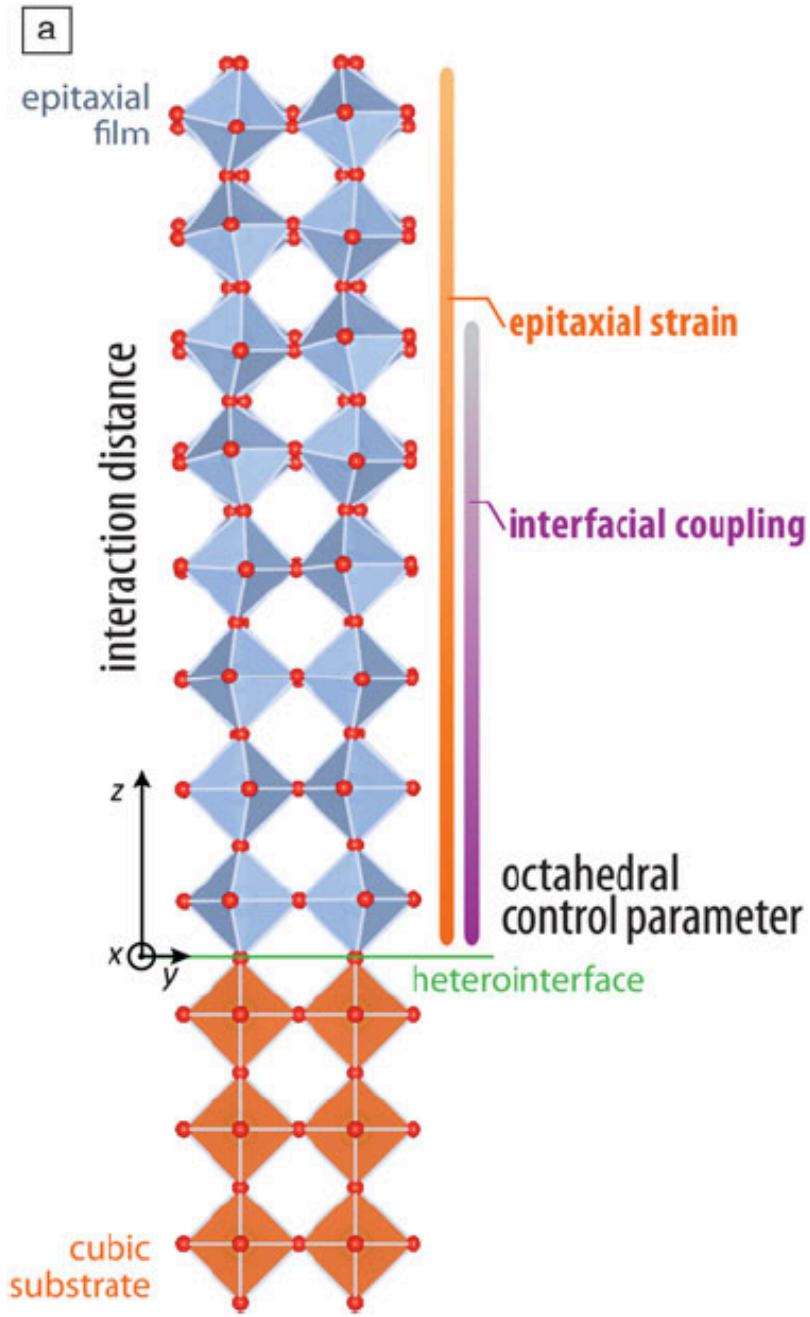
$Y_{2.24}Ba_{2.28}Ca_{3.48}Fe_{7.44}Cu_{0.56}O_{21}$

Predicted structure close to synthesized one



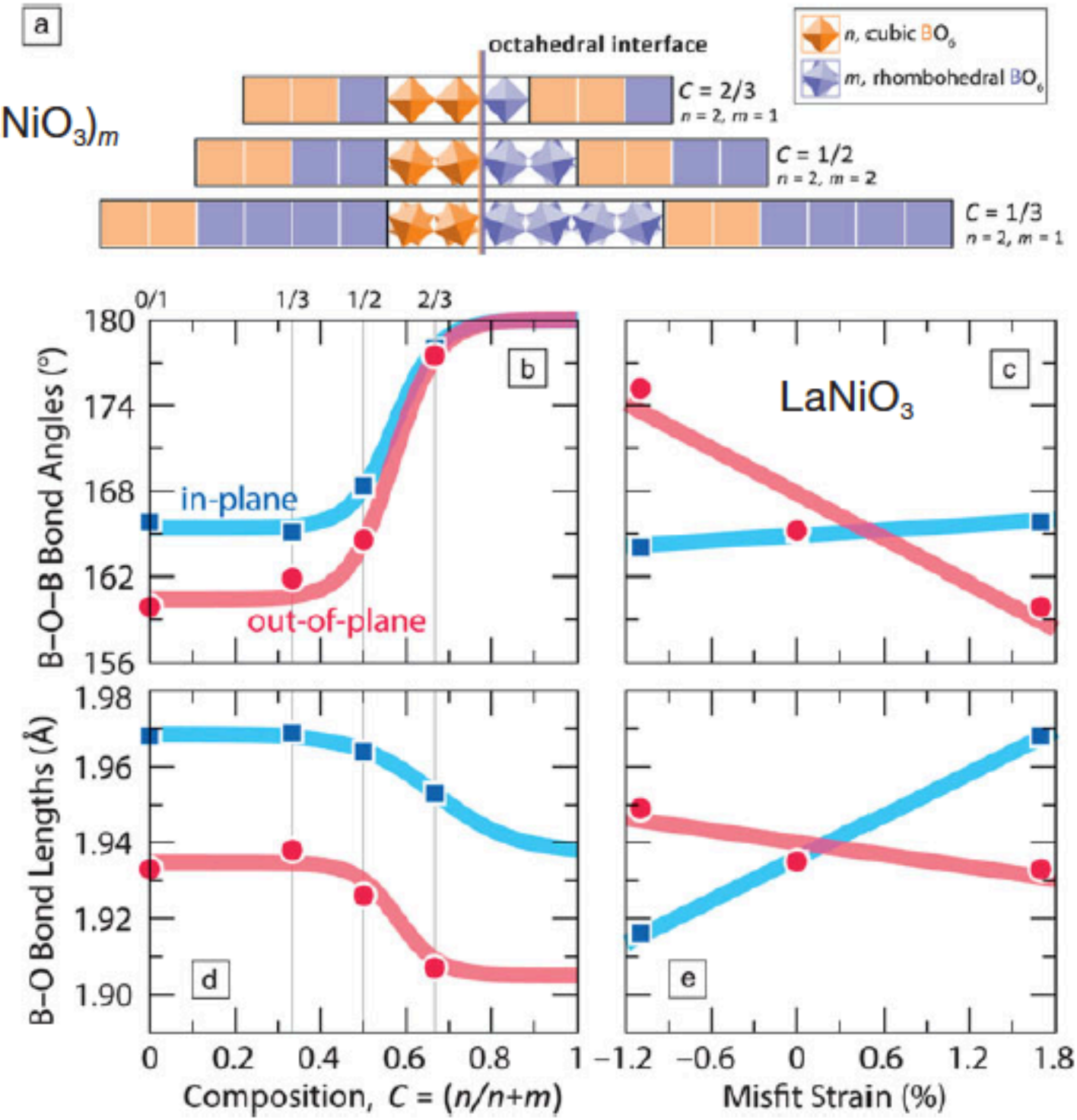
Octahedral Engineering



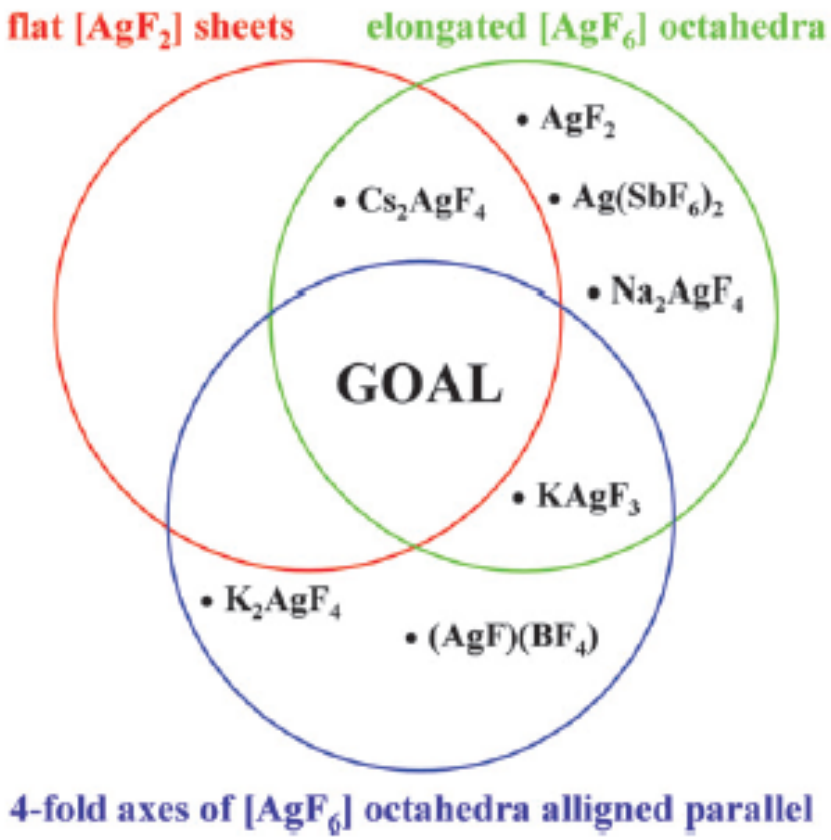


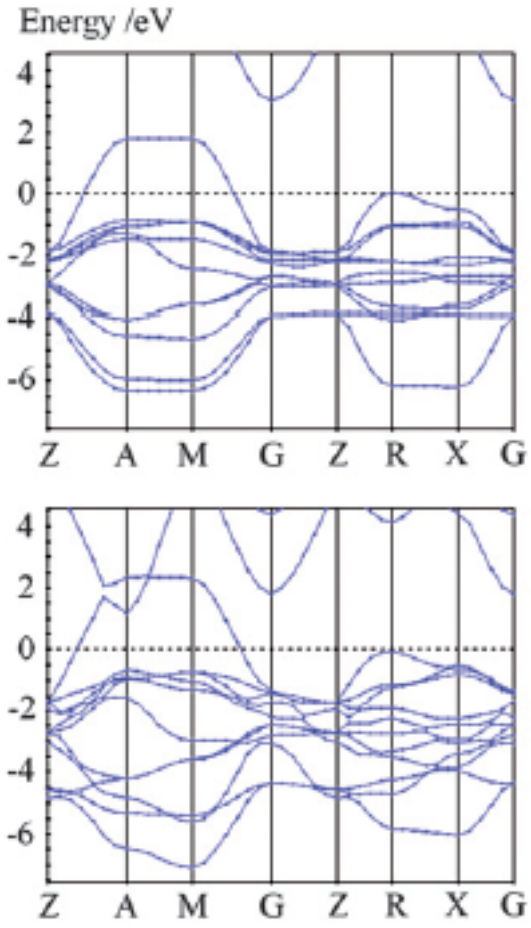
Rondinelli, May & Freeland, MRS Bulletin (2012)

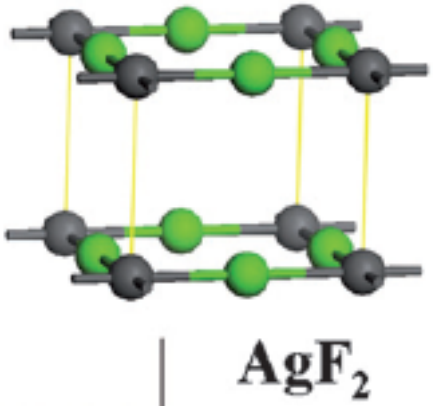
$(SrMnO_3)_n/(LaNiO_3)_m$

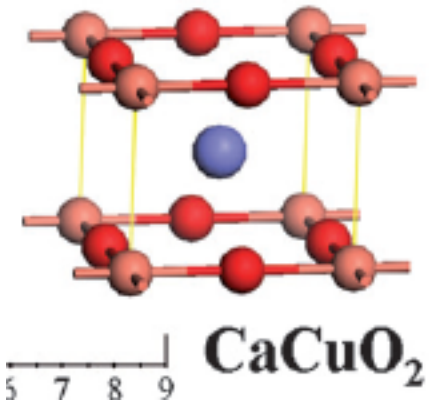


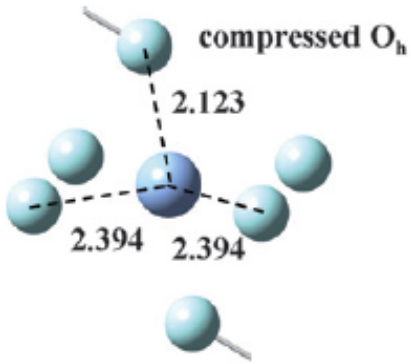
Quantum Chemical Considerations – Silver Flourides











$Ag(BF_4)_2(FH)_4$

Grochala, J. Mater. Chem. (2009)