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Desnity Functional Theory for Superconductors and its Application to Layered Nitride Superconductors

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Density functional theory for superconductors and its application to layered nitride superconductors

Ryotaro Arita (Univ. Tokyo)

Collaborators
Ryosuke Akashi
Kazuma Nakamura
Masatoshi Imada

ariXiv:1203.6487, to appear in PRB

Outline

- Layered nitride superconductors
  - T_c^{max}~26K
  - Pairing mechanism: conventional or unconventional ?
- DFT for superconductivity (SCDFT)
  - Formalism free from empirical parameters (such as μ^* in the Migdal-Eliashberg theory)
  - Successful for conventional superconductors: "Litmus paper" to determine whether the pairing mechanism is conventional or unconventional
- Application of SCDFT to layered nitrides
  - Unconventional SC ?

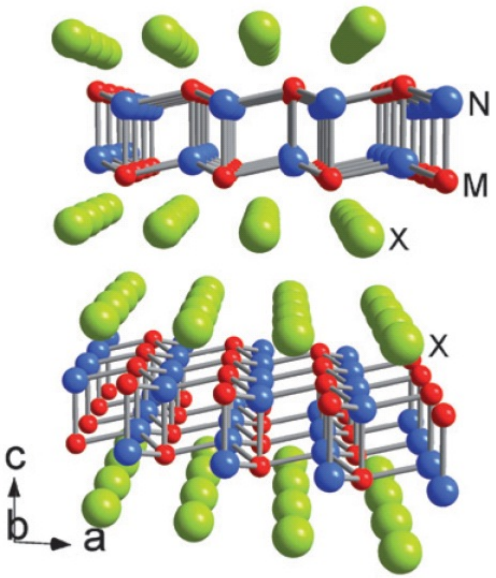
Layered nitride superconductors

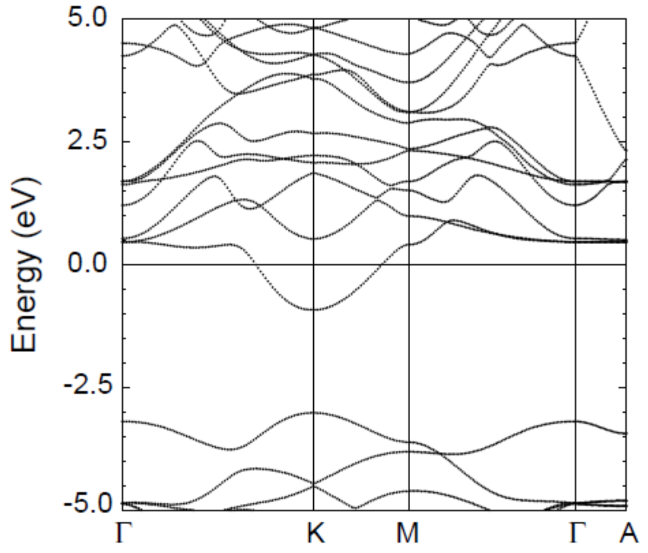
R. Weht *et al.*, Europhys. Lett., 48 320 (1999)

MNX

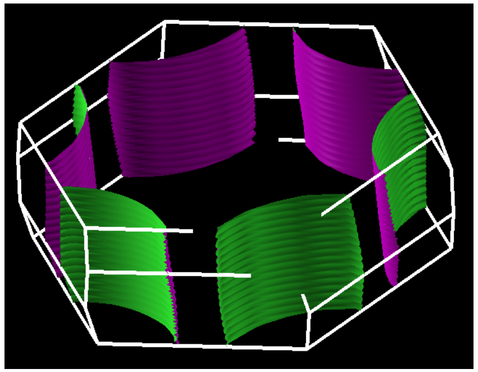
M=Ti, Zr, Hf

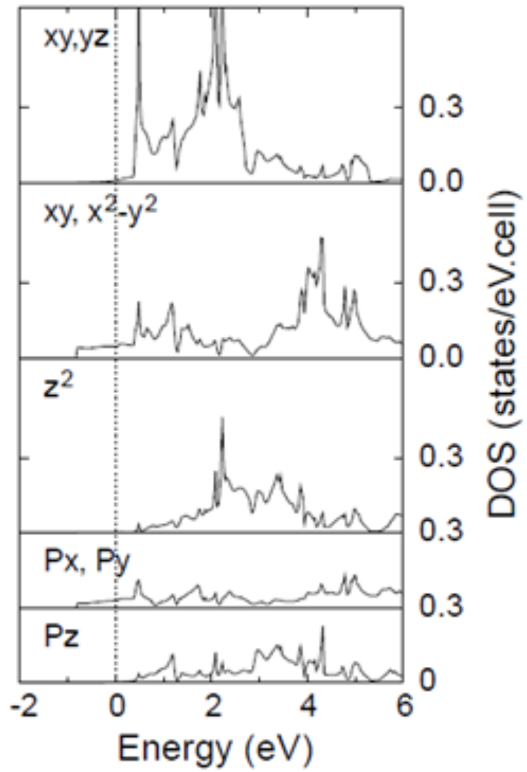
X= Cl, Br, I





Band structure of $Na_{0.25}HfNCl$.





2D electronic structure → constant DOS around E_F

Discovery of high T_c SC in layered ZrNCl

A New Layer-Structured Nitride Superconductor. Lithium-Intercalated β-Zirconium Nitride Chloride, Li_xZrNCl**

By *Shoji Yamanaka*,* *Hitoshi Kawaji*, *Ken-ichi Hotehama*, and *Masao Ohashi*

Adv. Mater. 8 771 (1996)

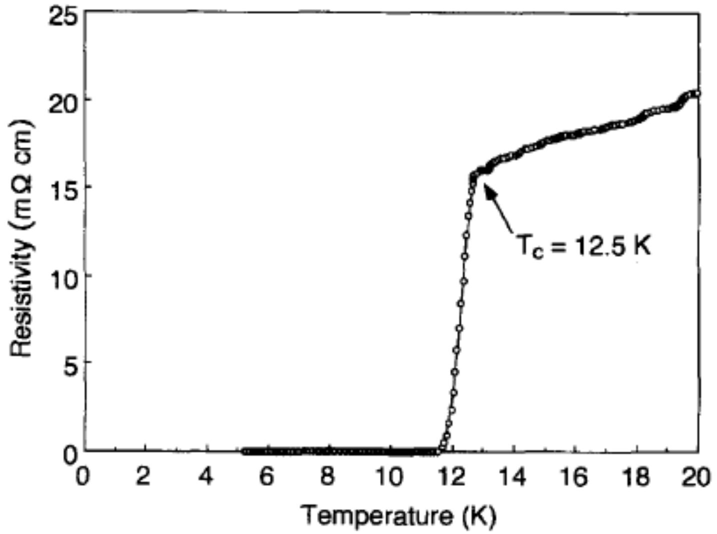


Fig. 3. Temperature dependence of the electrical resistivity of Li_xZrNCl.

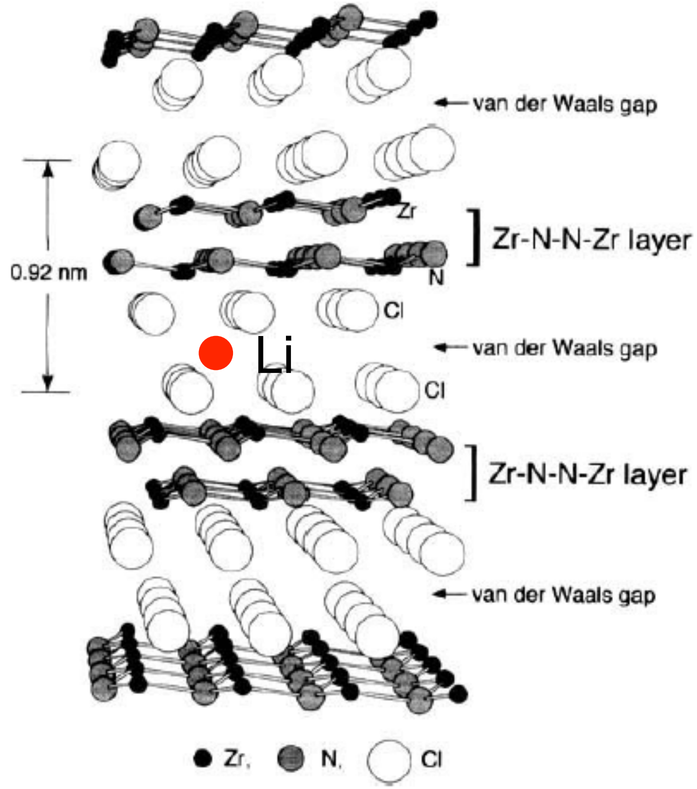
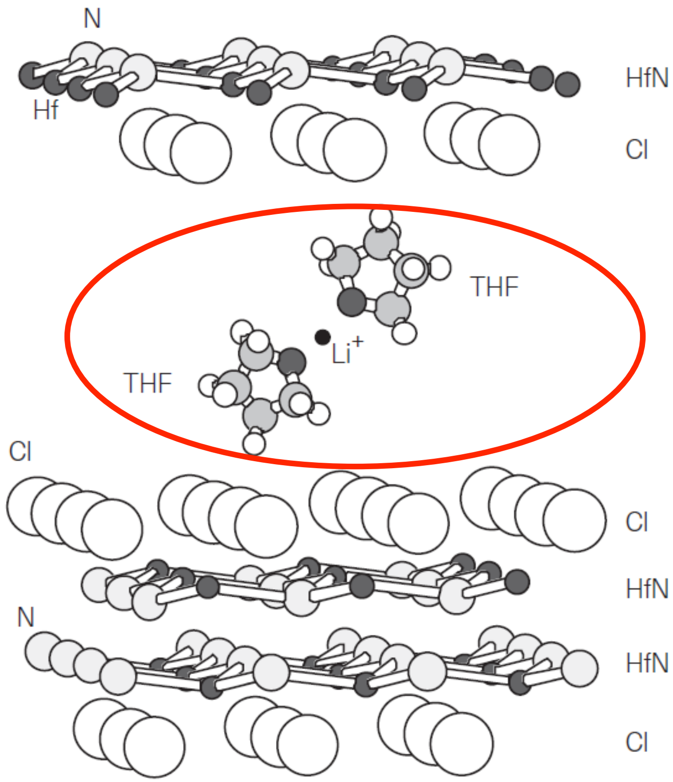


Fig. 1. Structure of β-ZrNCl.

Discovery of high T_c SC in layered nitrides

THE UNIVERSITY OF TOKYO

Band insulator exhibits superconductivity by co-intercalation of solvent molecules with alkali metals

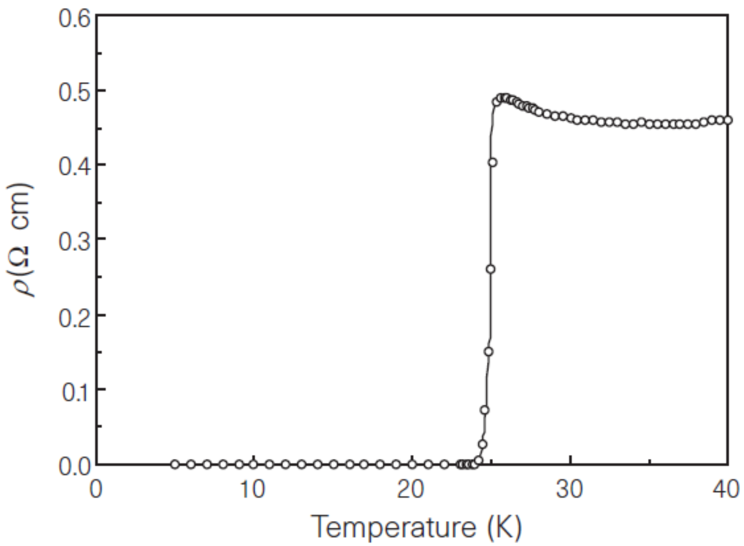


Superconductivity at 25.5 K in electron-doped layered hafnium nitride

Shoji Yamanaka*†, Ken-ichi Hotehama* & Hitoshi Kawaji*

** Department of Applied Chemistry, Faculty of Engineering, Hiroshima University, Higashi-Hiroshima 739, Japan*
† CREST, Japan Science and Technology Corporation (JST)

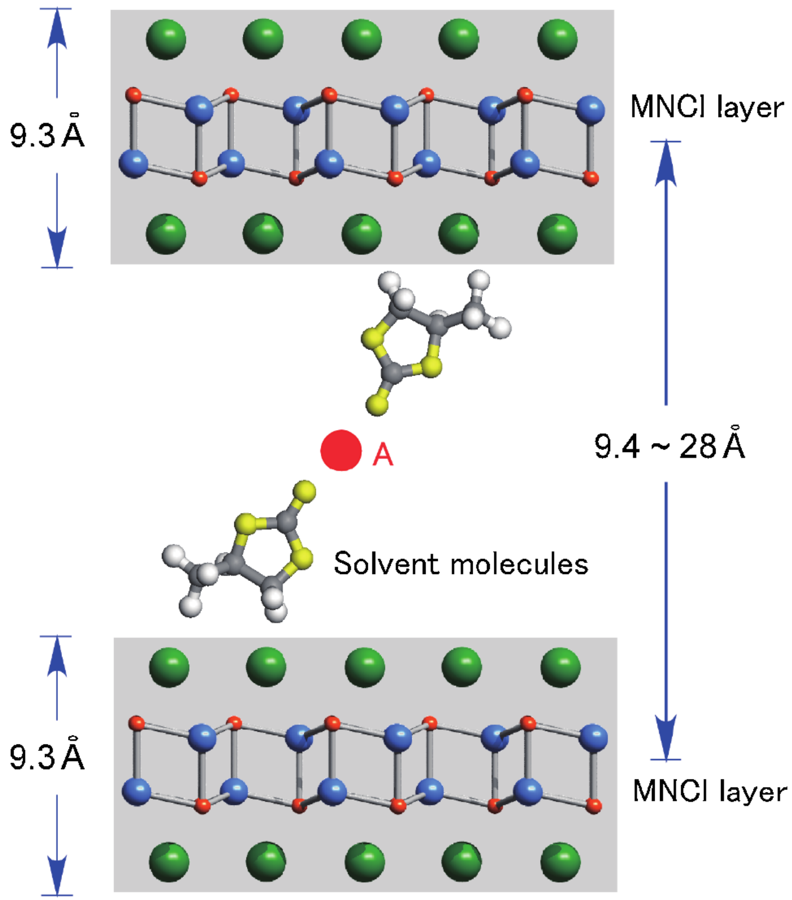
Nature 392 580 (1998)



Co-intercalation

Doping level & separation of the nitride layers: controllable by the co-intercalation of solvent molecules with alkali metals

Keeping the amount of carriers, the dimensionality of the system can be controlled



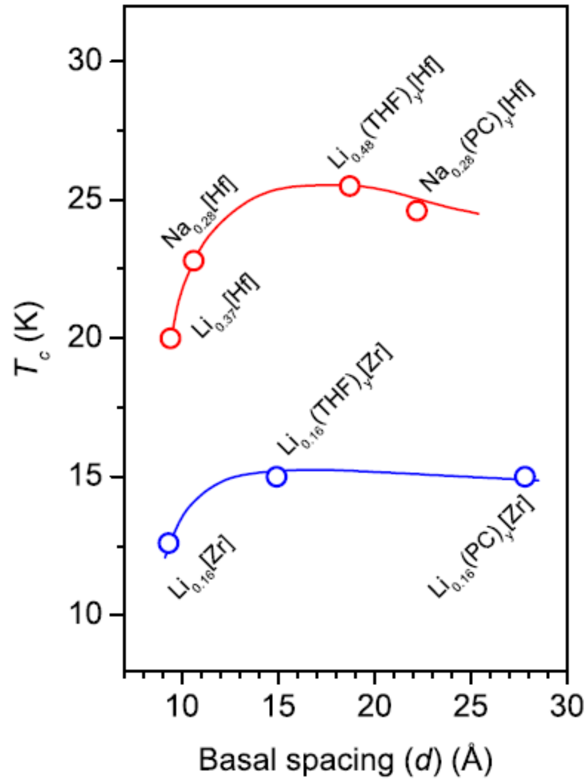
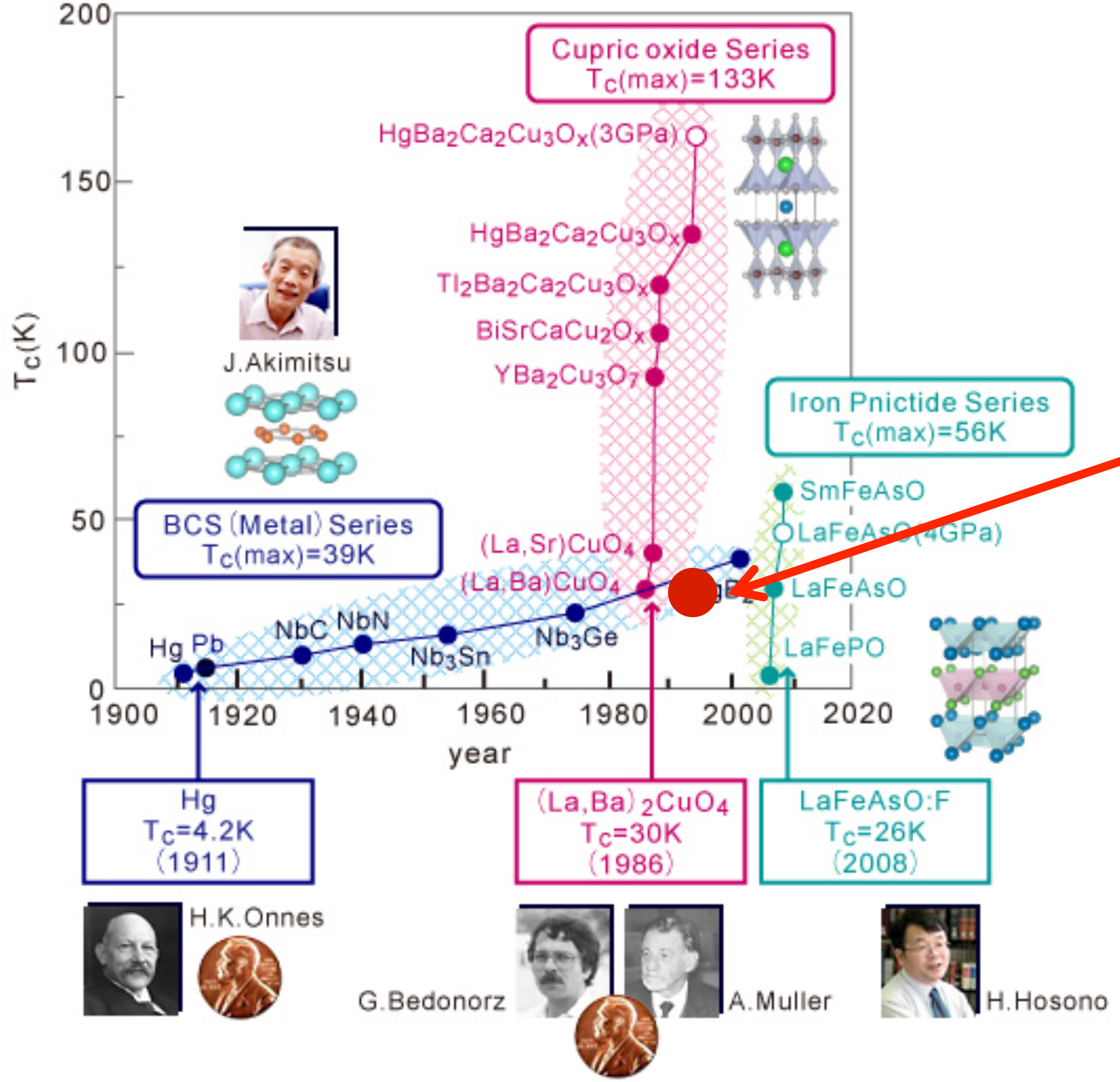


Fig. 6. (Color online) T_c vs the basal spacing (d) of the superconductors derived from β-ZrNCl ([Zr]) and HfNCl ([Hf]).

Hotehama et al, JPSJ 79 014707 (2010)

Record of High Tc

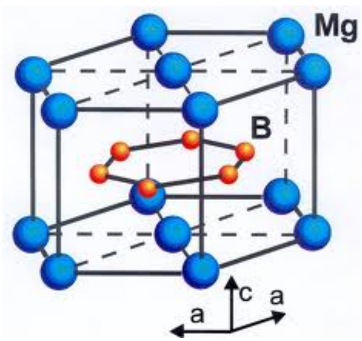


HfNCl

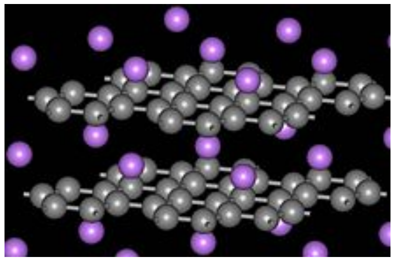
Experimental difficulties:
- Air sensitive
- Difficult to make single phase samples

http://www.supera.titech.ac.jp/research/index.html

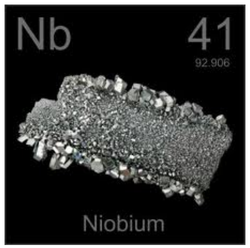
Conventional or Unconventional ?



MgB_2

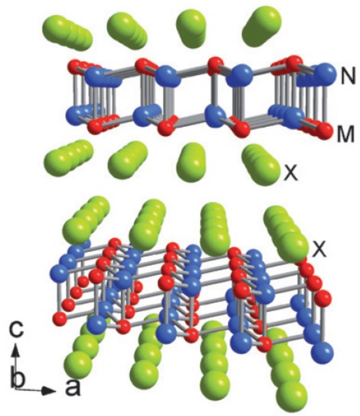


CaC_6

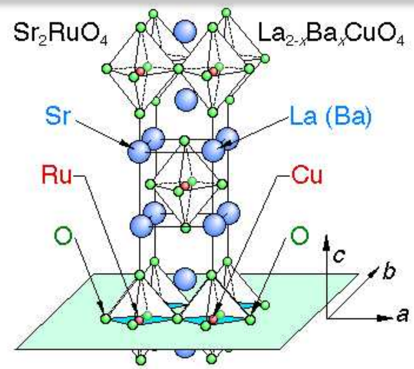


Simple metals

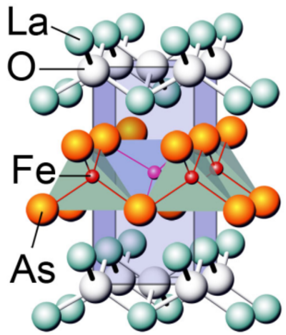
?



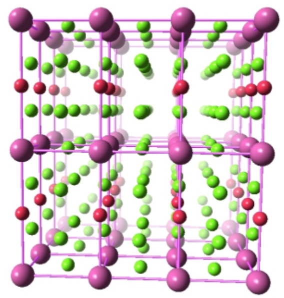
Nitrides



Cuprates / Ruthenates

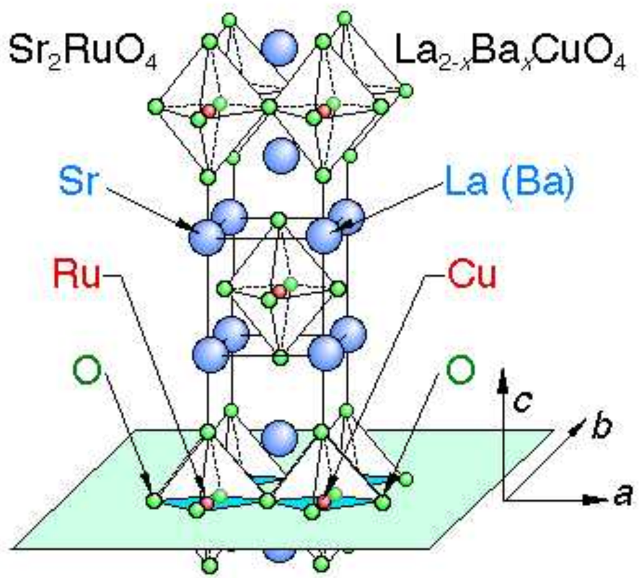


LaFeAsO

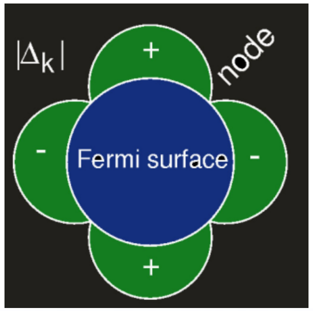


$CeRhIn_5$

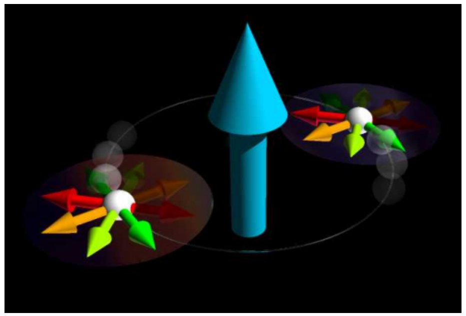
Unconventional SC



- High T_c cuprates: sign change in Δ

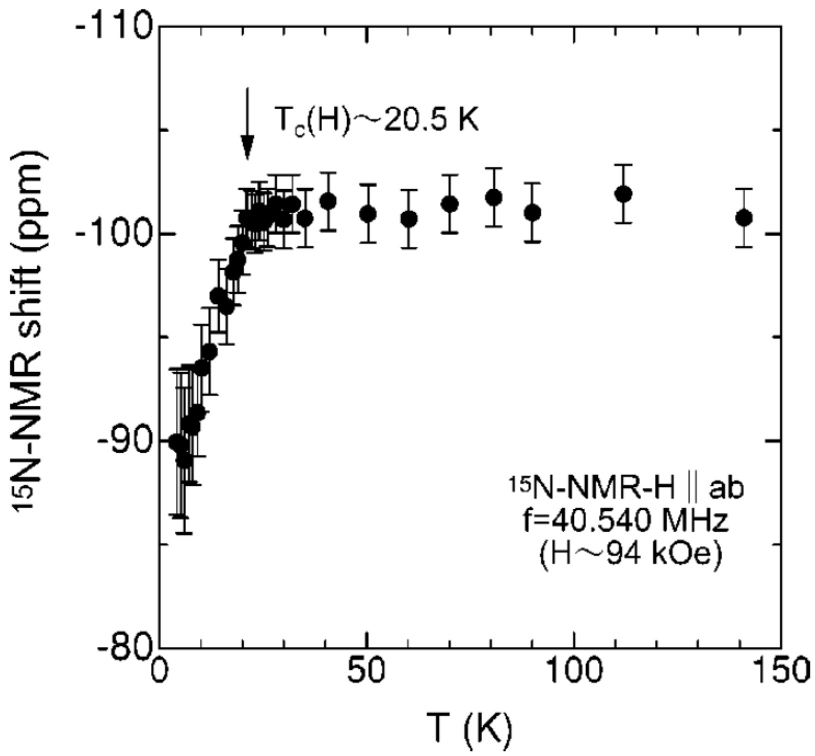


- Sr_2RuO_4 : spin triplet pairing



NMR

Tou *et al*., PRB 67 100509 (2003)

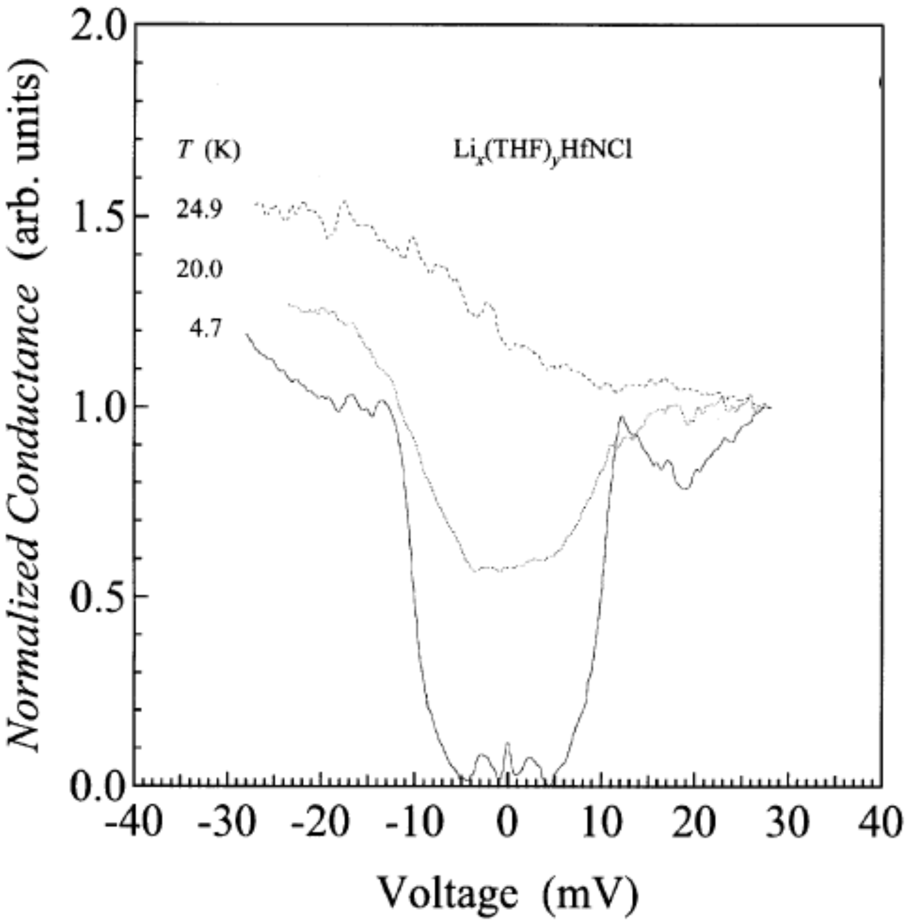


Knight shift decreases toward zero below T_c

Even parity, spin singlet pairing

STM/STS

T. Ekino *et al.*, Physica B 328 (2003) 23

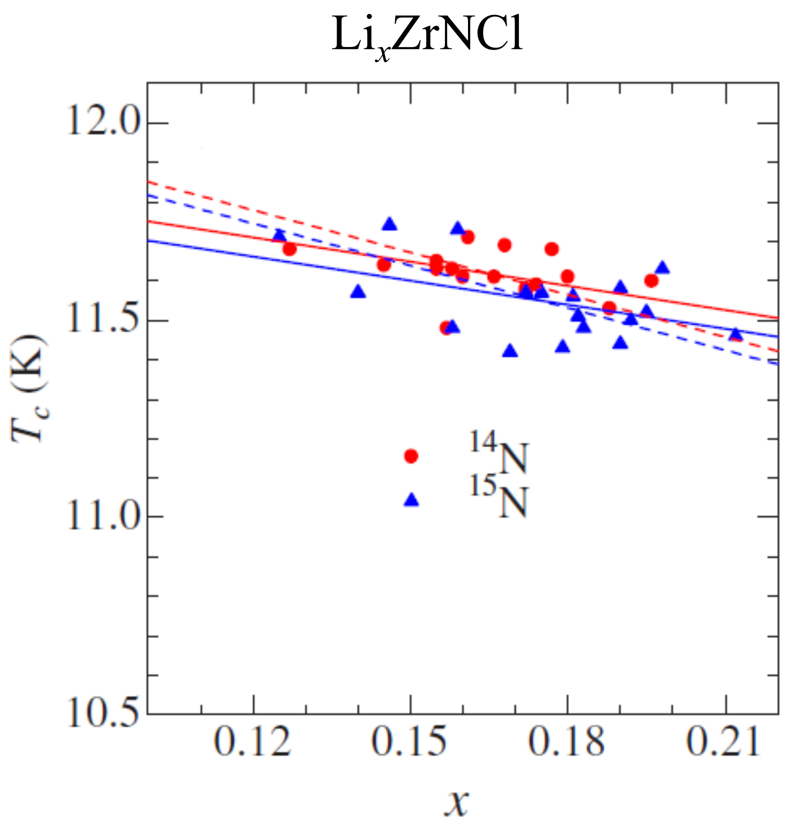


Temperature variation of the tunneling conductance

Full gap superconductivity

Isotope effect

Taguchi *et al.*, PRB 76 064508 (2007)



$\Delta T_c/T_c$ = -0.5 ±0.3 %
α_N=0.07±0.04

Unconventional SC ?

Static magnetic susceptibility

H. Tou *et al.*, PRL 86 5775 (2001)

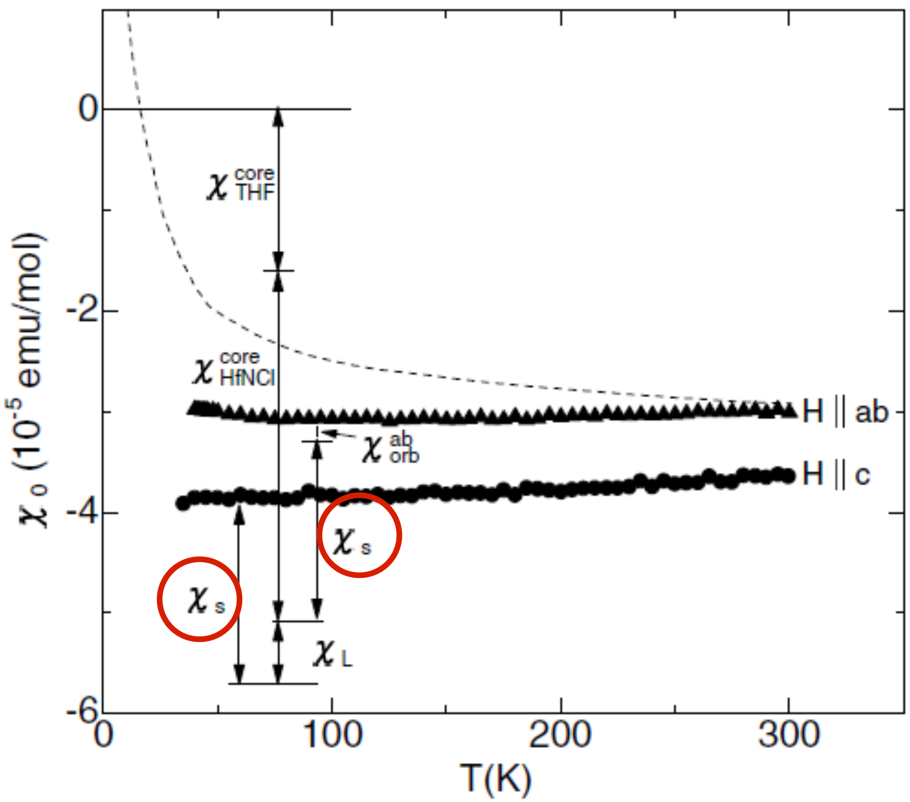


FIG. 2. Temperature dependence of susceptibility of $Li_{0.48}$-$(THF)_{0.3}HfNCl$ for $H \parallel c$ (circles) and $H \parallel ab$ (triangles). The dashed curve is the susceptibility of β-HfNCl.

Pauli susceptibility
~ 1.7 ×10 $^{-5}$ emu/mol

Small DOS(E_F)

Unconventional SC ?

Specific heat

Taguchi *et al.*, PRL 94 217002 (2005)

$$\Delta\gamma \equiv \left[C(H,T) - C(H=5\mathrm{T},T)\right]/T = AT^{-5/2}\exp(-\Delta_0/k_B T) - \gamma_n$$

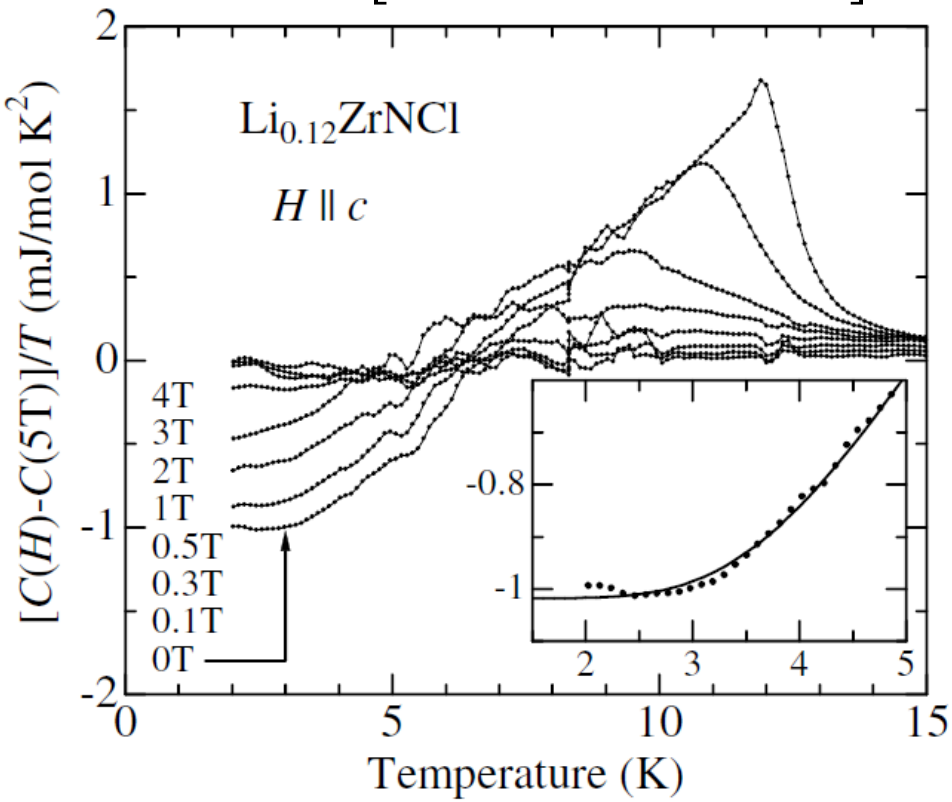


FIG. 3. Temperature dependence of the difference in the electronic specific coefficient between the superconducting state and the normal state for several H values. The inset shows the low-temperature behavior of $H = 0$ T data, together with the fit (solid line).

Specific heat coefficient (normal state)
γ_n=1.0 ± 0.1 mJ/mol K^2

$$\gamma_n = \frac{2}{3}(1+\lambda)\pi^2 k_B^2 N_{LDA}(0)$$

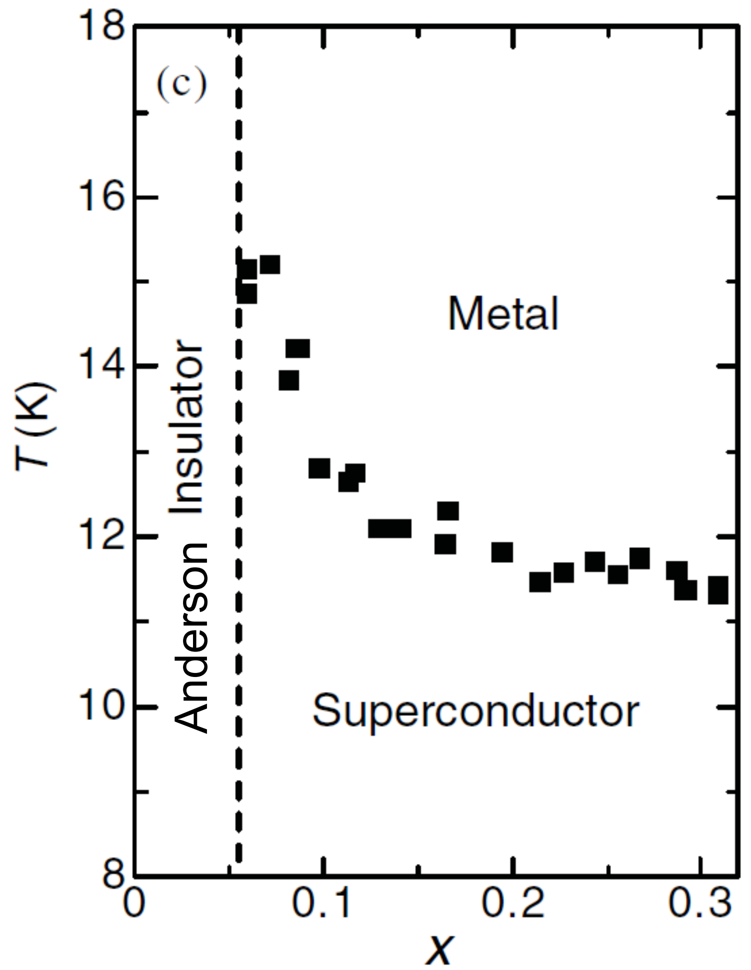
Mass enhancement
λ ~ 0.22

Strong-coupling gap ratio:
$2\Delta/k_B T_c$ = 4.6 ~ 5.2

Doping effect

Taguchi, *et. al*., PRL 97, 107001 (2006)

Li_xZrNCl



Increase in T_c for x <0.12

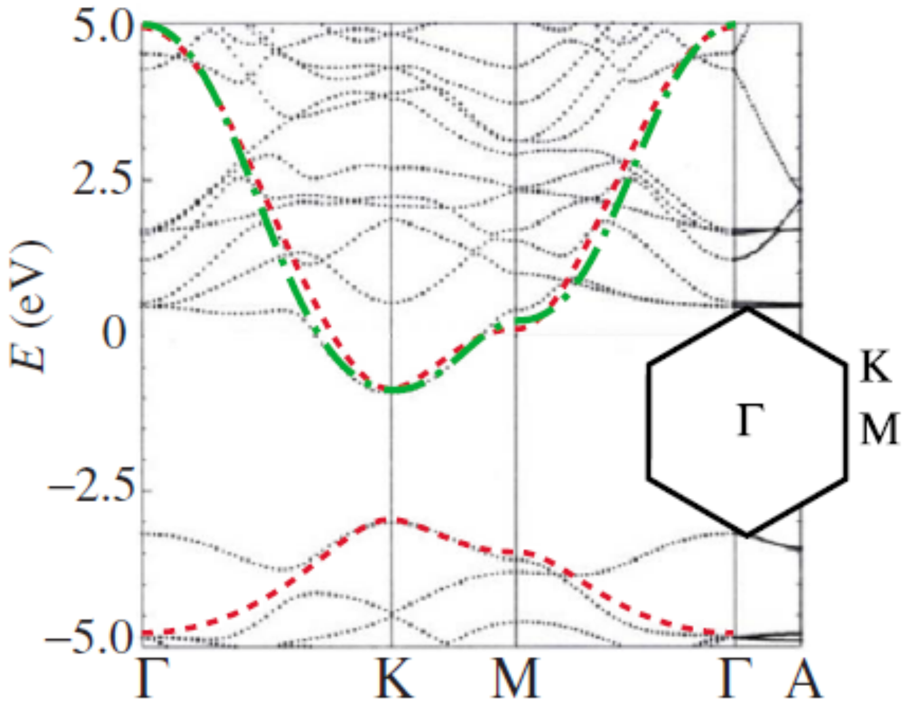
Unconventional SC ?

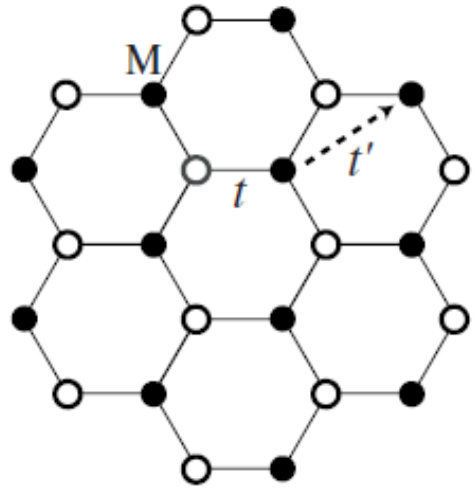
Unconventional scenario proposed so far

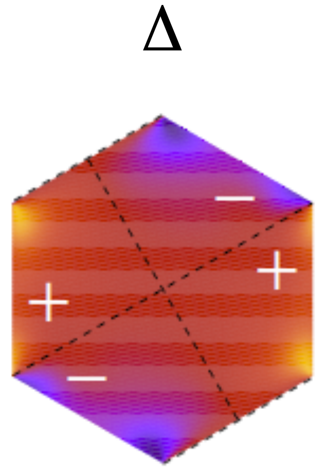
Spin-fluctuation-mediated *d+id* pairing

K. Kuroki, PRB 81 104502 (2010)

FLEX analysis for the 2-orbital Hubbard model







Unconventional scenario proposed so far

Dynamical screening and superconducting state in intercalated layered metallochloronitrides

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V. Z. Kresin
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(Received 26 April 2002; published 3 September 2002)

An essential property of layered systems is the dynamical nature of the screened Coulomb interaction. Low-energy collective modes appear as a consequence of the layering and provide for a superconducting-pairing channel in addition to the electron-phonon-induced attractive interaction. We show that taking into account this feature allows to explain the high critical temperatures ($T_c \sim 26$ K) observed in recently discovered intercalated metallochloronitrides. The exchange of acoustic plasmons between carriers leads to a significant enhancement of the superconducting critical temperature that is in agreement with the experimental observations.

Touchstone for Migdal-Eliashberg theory

McMillan's formula for T_c

$$T_c = \frac{\omega_{\ln}}{1.2} \exp\left[-\frac{1.04(1+\lambda)}{\lambda - \mu^*(1+0.62\lambda)} \right]$$

agrees with experimental T_c ?

McMillan's formula for T_c

$$T_c = \frac{\omega_{\ln}}{1.2} \exp\left[-\frac{1.04(1+\lambda)}{\lambda - \mu^*(1+0.62\lambda)} \right]$$

Logarithmic averaged frequency

$$\omega_{\ln} = \exp\left(\frac{2}{\lambda} \int_0^\infty d\omega \frac{\alpha^2 F(\omega)}{\omega} \ln(\omega) \right)$$

Ele-ph coupling

$$\lambda = 2 \int_0^\infty d\omega \frac{\alpha^2 F(\omega)}{\omega}$$

$$\alpha^2 F(\omega) = \frac{1}{2\pi N(E_F)} \sum_{\mathbf{q}\lambda} \frac{\gamma_{\mathbf{q}\lambda}}{\omega_{\mathbf{q}\lambda}} \delta(\omega - \omega_{\mathbf{q}\lambda})$$

$$\gamma_{\mathbf{q}\lambda} = 2\pi\omega_{\mathbf{q}\lambda} \sum_{\mathbf{k}\nu\nu'} |g^{\mathbf{q}\lambda}_{\mathbf{k}+\mathbf{q}\nu',\mathbf{k}\nu}|^2 \delta(\epsilon_{\mathbf{k}\nu}) \delta(\epsilon_{\mathbf{k}+\mathbf{q}\nu'})$$

$$g^{\mathbf{q}\lambda}_{\mathbf{k}+\mathbf{q}\nu',\mathbf{k}\nu} = \langle \mathbf{k}+\mathbf{q}\nu' | \delta^{\mathbf{q}\lambda} V_{\text{eff}} | \mathbf{k}\nu \rangle$$ Electron-phonon matrix element

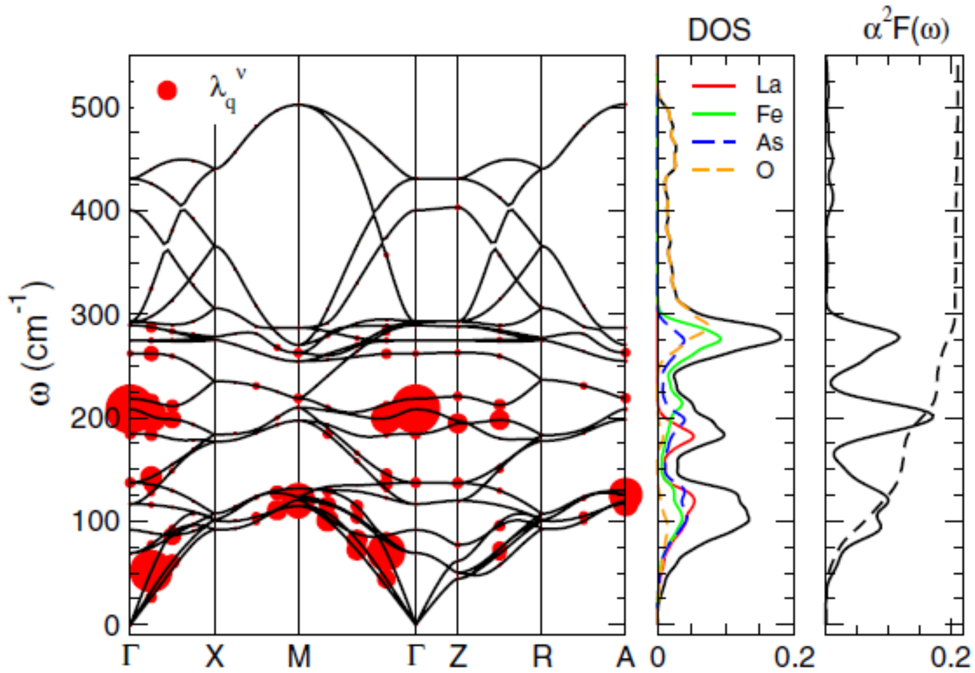
$\omega_{\mathbf{q}\lambda}$ Frequency of phonon

Coulomb pseudopotential

$$\mu^* = \frac{\mu}{1 + \mu \ln\left(\frac{E_F}{\omega_D} \right)}$$

Usually, treated as an empirical, adjustable parameter

Application of McMillan's formula to LaFeAsO

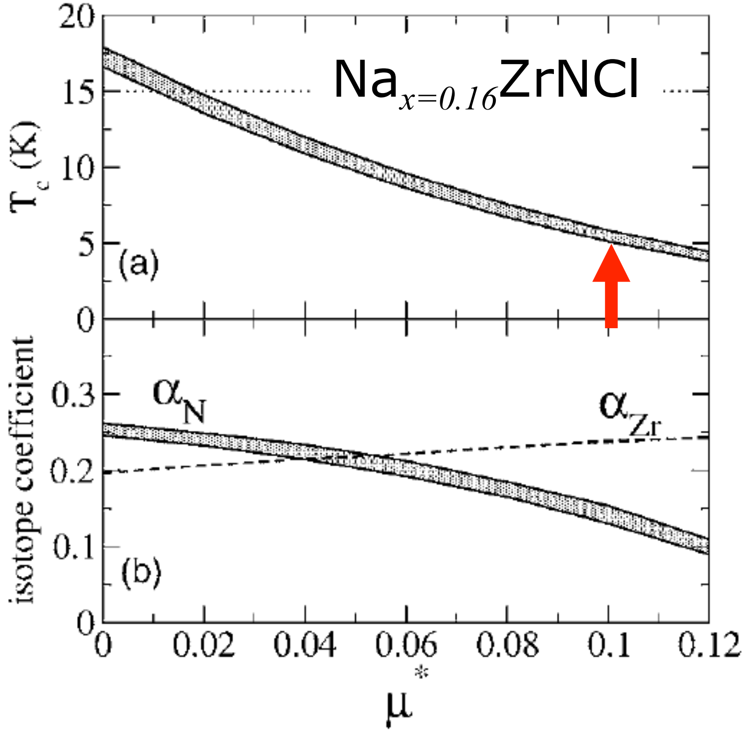


The total e-ph coupling constant λ, obtained by numerical integration of $\lambda(\Omega)$ up to $\omega = \infty$, is 0.21; this, together with a logarithmically averaged frequency $\omega_{\ln} = 205$ K, and $\mu^* = 0$, gives $T_c = 0.5$ K as an upper bound for T_c,

Boeri *et al.*, Phys. Rev. Lett. 101, 026403 (2008)

Standard Eliashberg study for nitrides

Heid, *et. al.*, PRB 72, 134527 (2005)



Yin-Kutepov-Kotliar, arXiv:1110.5751

Compounds	T_c(LDA/GGA)	T_c (HSE)	T_c (exp.)
ZrNCl	6.0	15.7	16 [29]
HfNCl	–	25.2	25.5 [10]
TiNCl	–	14.7	16.5 [28]

$\mu^*=0.1$

Can we examine ME theory without μ^* ?

↓

<u>SCDFT</u>

DFT for normal state

$$\hat{H}_e = \hat{T}_e + \hat{W}_{ee} + \int \hat{\rho} v(r) \mathrm{d}^3 r$$

Hohenberg-Kohn theorem

$$v \longleftrightarrow \rho$$

one-to-one correspondence

Kohn-Sham equation

$$\left(-\frac{\nabla^2}{2} + v_s(r) - \mu \right) \phi_i(r) = E_i \phi_i(r) \qquad \rho(r) = \sum_j \left| \phi_j(r) \right|^2$$

$$v_s[\rho] = v_{ext} + v_H^{ee}[\rho] + v_{xc}[\rho] \qquad v_{xc} = \frac{\delta E_{xc}}{\delta \rho}$$

DFT for superconductors

Oliveira et al., PRL 60, 2430 (1988)
Kreibich & Gross PRL 86, 2984 (2001)

$$\hat{H}_e = \hat{T}_e + \hat{W}_{ee} + \int \hat{\rho} v(r) \mathrm{d}^3 r - \int \mathrm{d}^3 r \int \mathrm{d}^3 r' \left(\hat{\chi}(r, r') \Delta^*(r, r') + \mathrm{H.c.} \right)$$

$$\rho(r) = \left\langle \sum_{\sigma=\uparrow\downarrow} \hat{\psi}_\sigma^+(r) \hat{\psi}_\sigma(r) \right\rangle$$ electron density

$$\chi(r, r') = \left\langle \hat{\psi}_\uparrow(r) \hat{\psi}_\downarrow(r') \right\rangle$$ anomalous density

Hohenberg-Kohn theorem for superconductors

$$[v, \Delta] \longleftrightarrow [\rho, \chi]$$

Kohn-Sham BdG equation

M. Lüders et al, PRB 72, 024545 (2005), M. Marques et al, PRB 72, 024546 (2005)

$$\left(-\frac{\nabla^2}{2}+v_s(r)-\mu\right)u_i(r)+\int d^3r'\Delta_s(r,r')v_i(r')=E_iu_i(r)$$

$$-\left(-\frac{\nabla^2}{2}+v_s(r)-\mu\right)v_i(r)+\int d^3r'\Delta_s^*(r,r')u_i(r')=E_iv_i(r)$$

$$\begin{aligned}v_s[\rho,\chi](\mathbf{r}) &= v_{ext}+v_H^{ee}[\rho]+v_{xc}[\rho,\chi]\\ &= \int d\mathbf{r}'\frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}+\frac{\delta F_{xc}}{\delta\rho(\mathbf{r})}\end{aligned}$$

$$\begin{aligned}\Delta_s[\rho,\chi](\mathbf{r},\mathbf{r}') &= \Delta_{ext}+\Delta_H+\Delta_{xc}\\ &= -\frac{\chi(\mathbf{r},\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}+\frac{\delta F_{xc}}{\delta\chi^*(\mathbf{r},\mathbf{r}')}\end{aligned}$$

Gap equation

M. Lüders et al, PRB 72, 024545 (2005), M. Marques et al, PRB 72, 024546 (2005)

Linearized gap equation

$$\Delta_i = \frac{-1}{2} \sum_j F_{ij}^{\mathrm{Hxc}} \frac{\tanh[\beta \xi_j / 2]}{\xi_j} \Delta_j$$

$$F_{ij}^{\mathrm{Hxc}} = \frac{\delta^2 (E_H + F_{xc})}{\delta \chi_i^* \delta \chi_j}$$

$$E_H = \frac{1}{2} \int d^3 r \int d^3 r' \frac{\rho(\mathbf{r}) \rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} + \int d^3 r \int d^3 r' \frac{|\chi(\mathbf{r}, \mathbf{r}')|^2}{|\mathbf{r} - \mathbf{r}'|}$$

If F_{xc} is given, we can calculate T_c

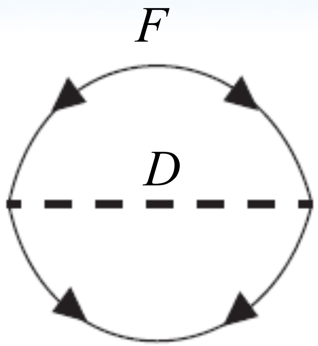
Exchange correlation functional F_{xc}

F_{xc}=phonon term + Coulomb term

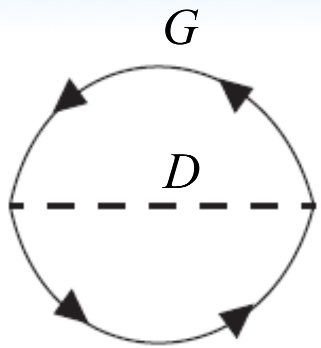
Let us first consider the phonon part in F_{xc}

Phonon contribution to F_{xc}

$F_{xc}{}^{a} =$



$F_{xc}{}^{b} =$



$$G^{s}_{\sigma,\sigma'}(\boldsymbol{r},\boldsymbol{r}';\omega_n) = \delta_{\sigma,\sigma'}\sum_i \left[\frac{u_i(\boldsymbol{r})u_i^*(\boldsymbol{r}')}{i\omega_n - E_i} + \frac{v_i(\boldsymbol{r})v_i^*(\boldsymbol{r}')}{i\omega_n + E_i} \right]$$

$$F^{s}_{\sigma,\sigma'}(\boldsymbol{r},\boldsymbol{r}';\omega_n) = \delta_{\sigma,-\sigma'}\mathrm{sgn}(\sigma') \times \sum_i \left[\frac{v_i^*(\boldsymbol{r})u_i(\boldsymbol{r}')}{i\omega_n + E_i} - \frac{u_i(\boldsymbol{r})v_i^*(\boldsymbol{r}')}{i\omega_n - E_i} \right]$$

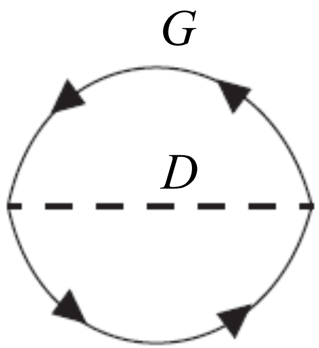
$$D^{s}_{\lambda,\boldsymbol{q}}(\nu_n) = -\frac{2\Omega_{\lambda,\boldsymbol{q}}}{\nu_n^2 + \Omega^2_{\lambda,\boldsymbol{q}}}$$

Phonon contribution to F_{xc}

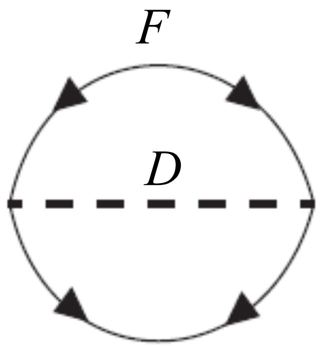
$$\Delta_i = \frac{-1}{2}\sum_j K_{ij}^{\mathrm{Hxc}} \frac{\tanh[\beta\xi_j/2]}{\xi_j}\Delta_j$$

$$K_{ij}^{\mathrm{Hxc}} = \frac{\delta^2 (E_H + F_{xc})}{\delta\chi_i^* \delta\chi_j}$$

$F_{xc}{}^{b} =$



$F_{xc}{}^{a} =$



$$\Delta_i = -Z_i\Delta_i - \frac{1}{2}\sum_j K_{ij}^{ph} \frac{\tanh[(\beta/2)\xi_j]}{\xi_j}\Delta_j$$

Comparison between SCDFT and ME

M. Lüders et al, PRB 72, 024545 (2005)

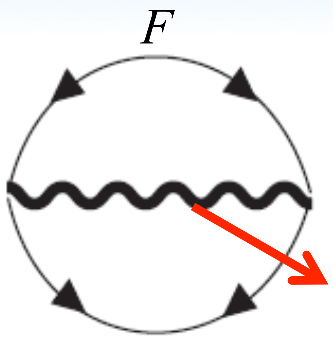
TABLE I. Transition temperatures from numerical solutions of the phonon-only DFT and Eliashberg equations. All temperatures are in kelvin.

	Al	Nb	Mo	Ta	V	Pb
$\mathcal{K}^{\rm ph}+\mathcal{Z}^{\rm ph}$	7.10	23.0	5.23	11.7	34.2	12.8
Eliashberg	9.75	24.7	7.31	14.0	36.4	12.2

For the phonon part, SCDFT ~ McMillan

Coulomb contribution to F_{xc}

$F_{xc}^{\,c} =$



RPA screened Coulomb $V_c(\omega=0)$

$$\Delta_i = -Z_i \Delta_i - \frac{1}{2}\sum_j \left(K_{ij}^{ph} + K_{ij}^{C}\right)\frac{\tanh[(\beta/2)\xi_j]}{\xi_j}\Delta_j$$

State dependent:
energy scale ~ω_D

Almost state independent

Retardation effect is represented in DFT
without introducing adjustable parameters like μ^*

Application to simple metals

M. Lüders et al, PRB 72, 024545 (2005), M. Marques et al, PRB 72, 024546 (2005)

Transition temperatures from DFT calculation

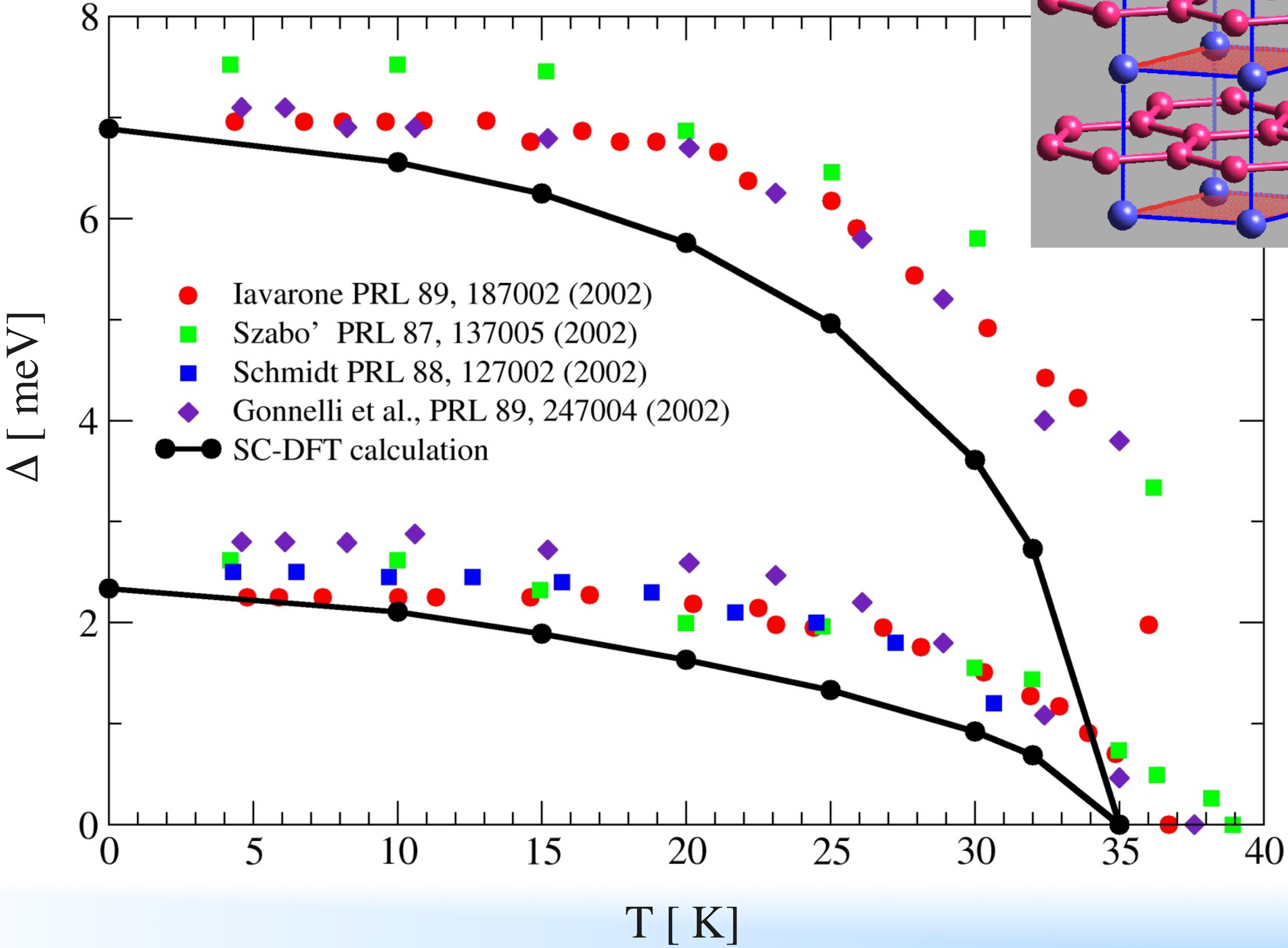
	Al	Nb	Ta	Pb	Cu
DFT	0.9	9.5	3.7	6.9	<0.01
Experimental	1.18	9.5	4.5	7.2	-

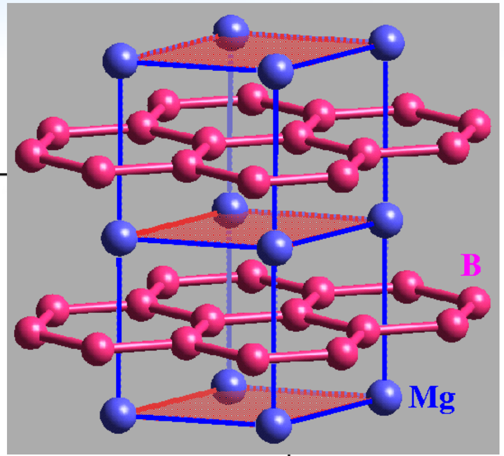
Gap at zero temperature

	Al	Nb	Ta	Pb	Cu
DFT	0.14	1.74	0.63	1.34	-
Experimental	0.179	1.55	0.69	1.33	-

Application to MgB_2

A. Floris et al, Phys. Rev. Lett. 94, 037004 (2005)

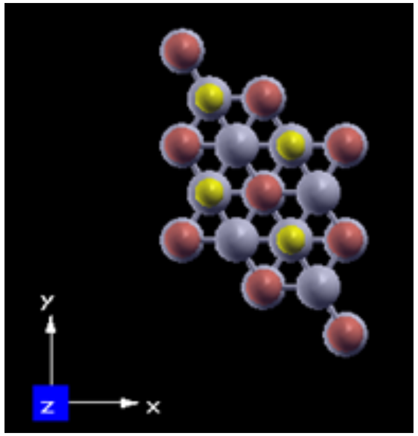


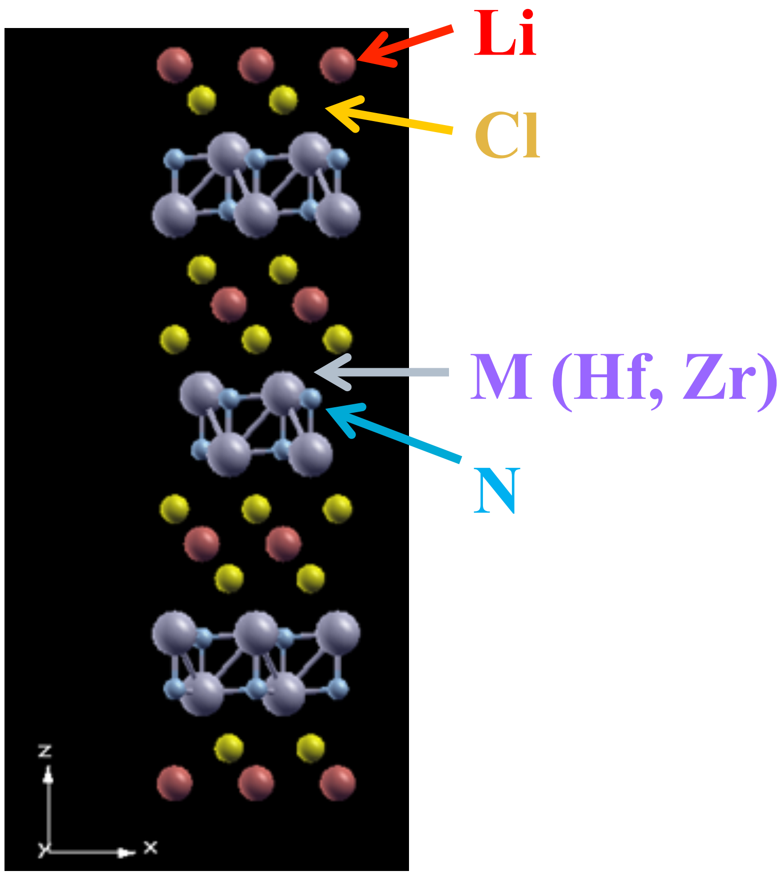


SCDFT= method without empirical parameters

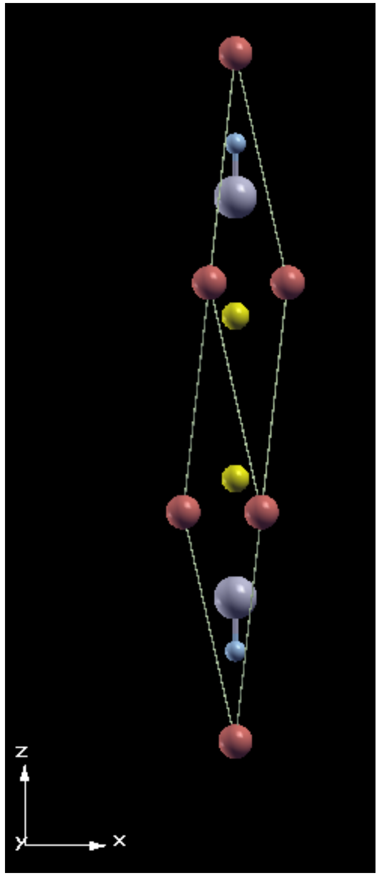
In the present study, we use SCDFT as a Litmus paper to determine whether the pairing mechanism of layered nitrides is conventional or unconventional

$Li_{0.5}MNCl$



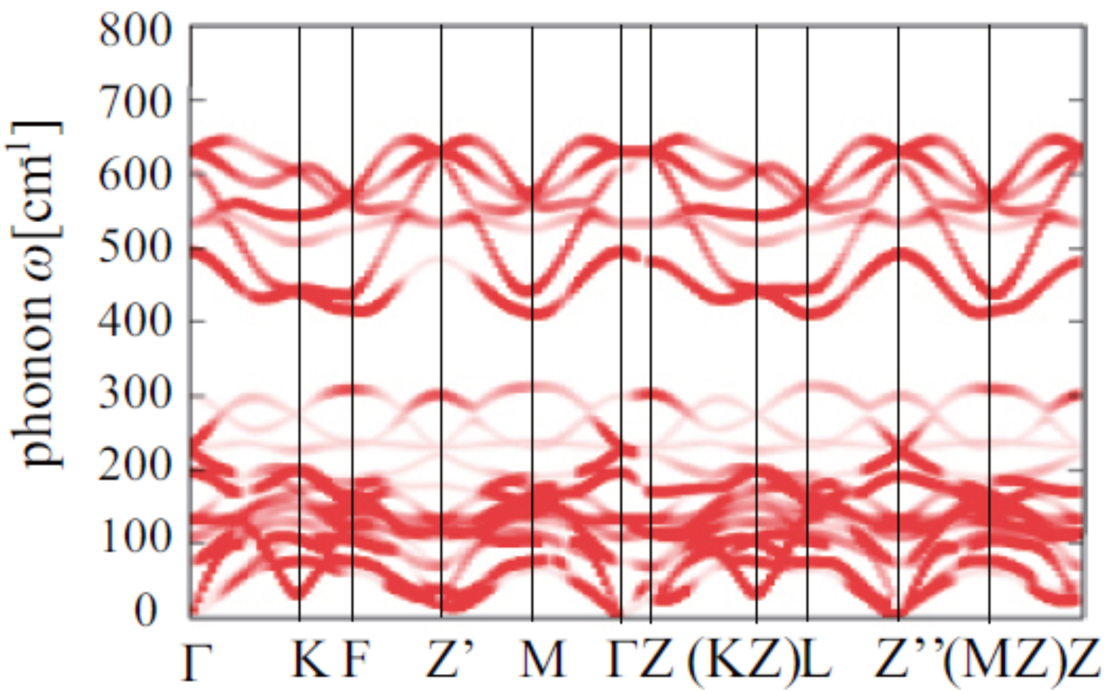


Unit cell



Result: phonon spectrum & ele-ph coupling

$Li_{0.5}HfNCl$



Ele-ph coupling

$$\lambda = 2\int_0^\infty d\omega \frac{\alpha^2 F(\omega)}{\omega} = 1.29$$

Logarithmic averaged frequency

$$\omega_{\ln} = \exp\left(\frac{2}{\lambda}\int_0^\infty d\omega \frac{\alpha^2 F(\omega)}{\omega}\ln(\omega)\right)$$

$=204$ [cm^{-1}]

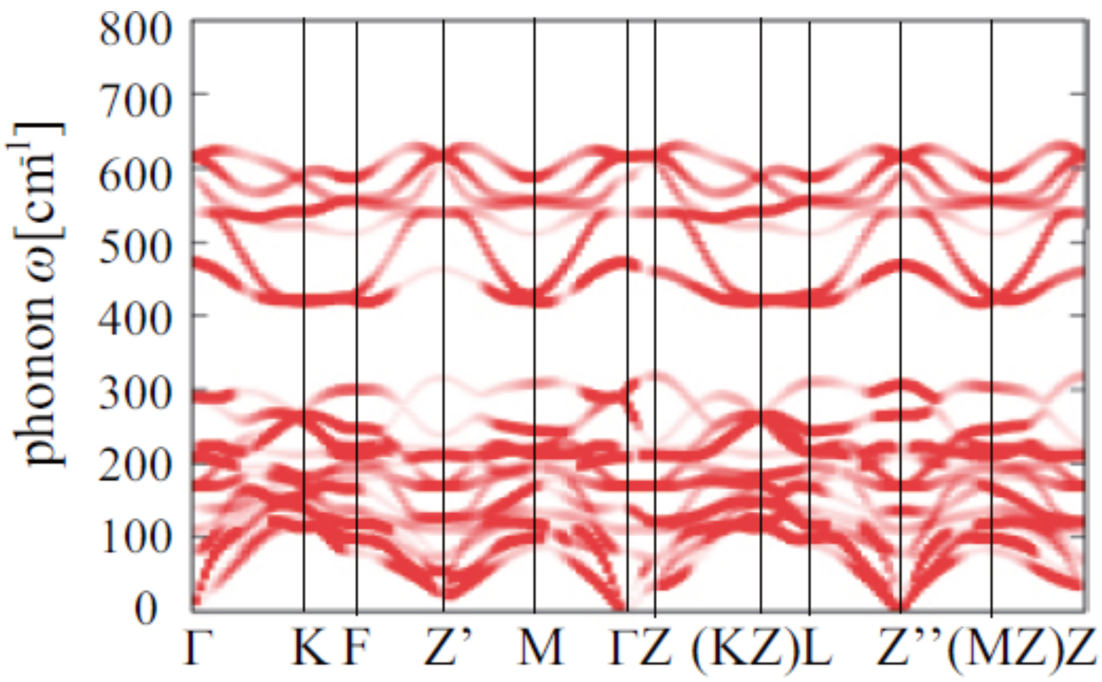
$$T_c = \frac{\omega_{\ln}}{1.2}\exp\left[-\frac{1.04(1+\lambda)}{\lambda}\right] = 26.9\text{K}$$

$$\gamma_{q\lambda} = 2\pi\omega_{q\lambda}\sum_{k\nu\nu'} |g^{q\lambda}_{k+q\nu',k\nu}|^2 \delta(\epsilon_{k\nu})\delta(\epsilon_{k+q\nu'})$$

$$\alpha^2 F(\omega) = \frac{1}{2\pi N(E_F)}\sum_{q\lambda}\frac{\gamma_{q\lambda}}{\omega_{q\lambda}}\delta(\omega - \omega_{q\lambda})$$

Result: phonon spectrum & ele-ph coupling

$Li_{0.5}ZrNCl$



Ele-ph coupling

$$\lambda = 2\int_0^\infty d\omega \frac{\alpha^2 F(\omega)}{\omega}$$ =0.98

Logarithmic averaged frequency

$$\omega_{\ln} = \exp\left(\frac{2}{\lambda}\int_0^\infty d\omega \frac{\alpha^2 F(\omega)}{\omega}\ln(\omega)\right)$$

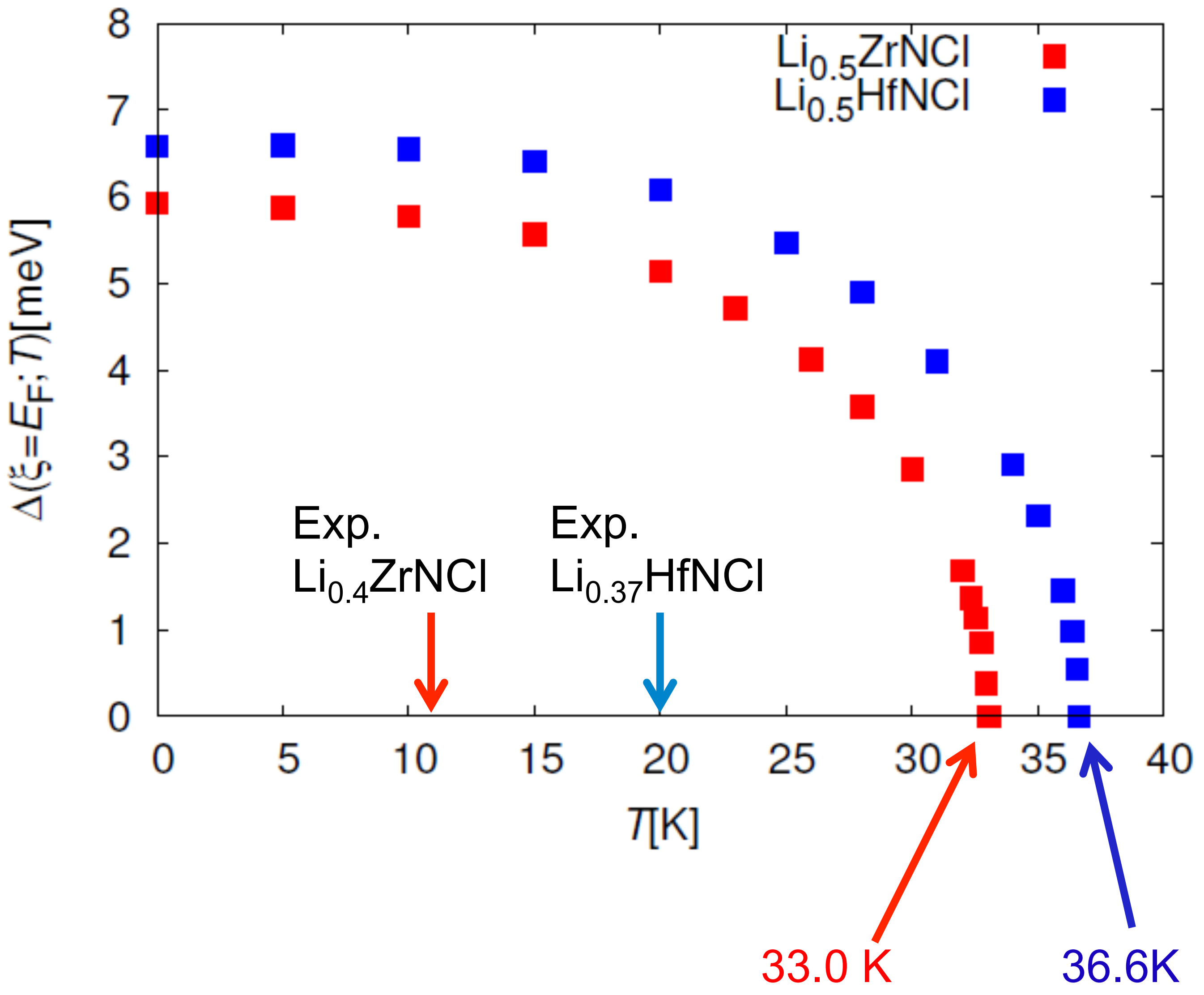
=304 [cm^{-1}]

$$T_c = \frac{\omega_{\ln}}{1.2}\exp\left[-\frac{1.04(1+\lambda)}{\lambda}\right] = 31.1\mathrm{K}$$

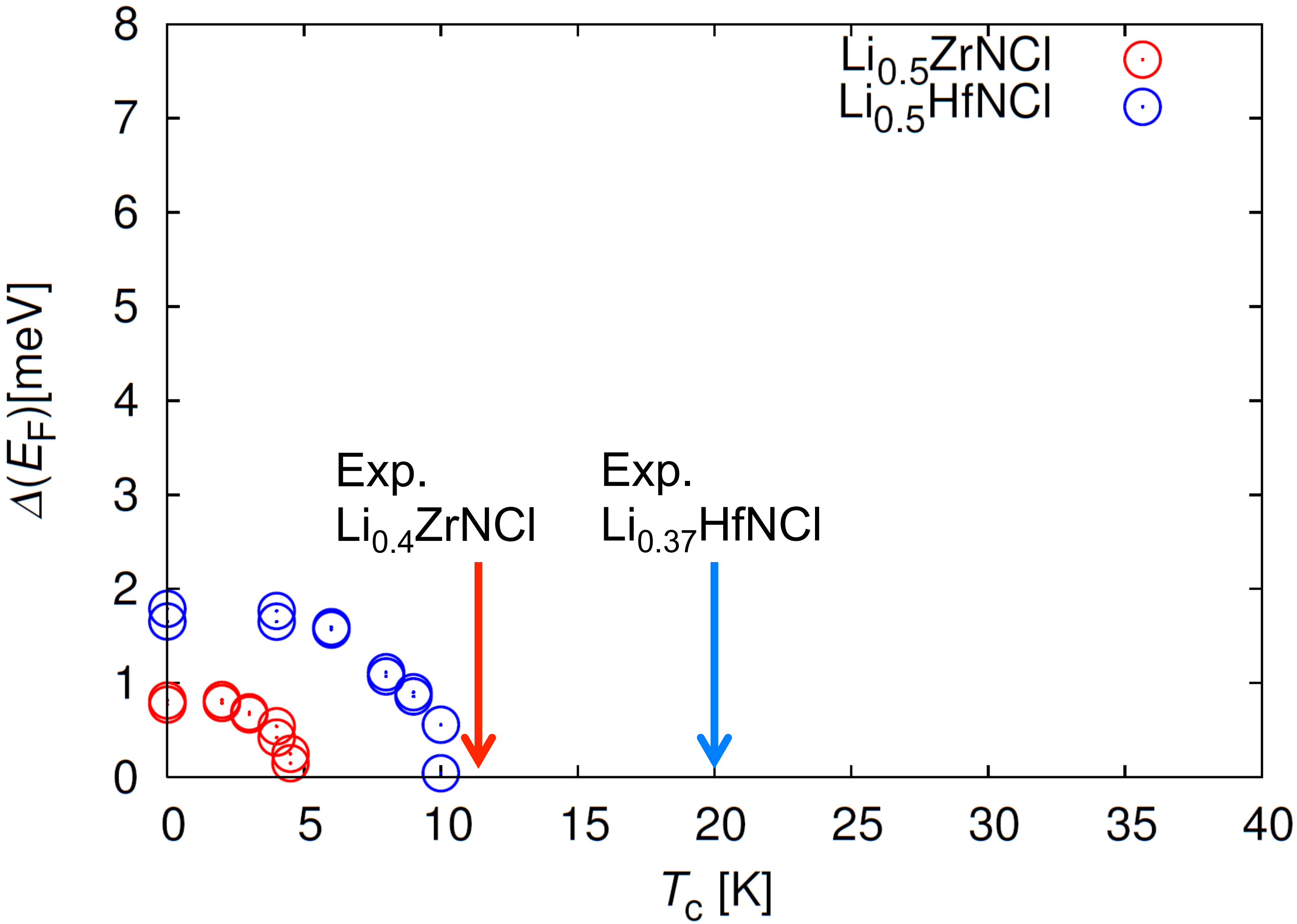
$$\gamma_{q\lambda} = 2\pi\omega_{q\lambda}\sum_{k\nu\nu'} |g^{q\lambda}_{k+q\nu',k\nu}|^2 \delta(\epsilon_{k\nu})\delta(\epsilon_{k+q\nu'})$$

$$\alpha^2 F(\omega) = \frac{1}{2\pi N(E_F)}\sum_{q\lambda}\frac{\gamma_{q\lambda}}{\omega_{q\lambda}}\delta(\omega-\omega_{q\lambda})$$

Result: calculation without F_{xc}^{ee}



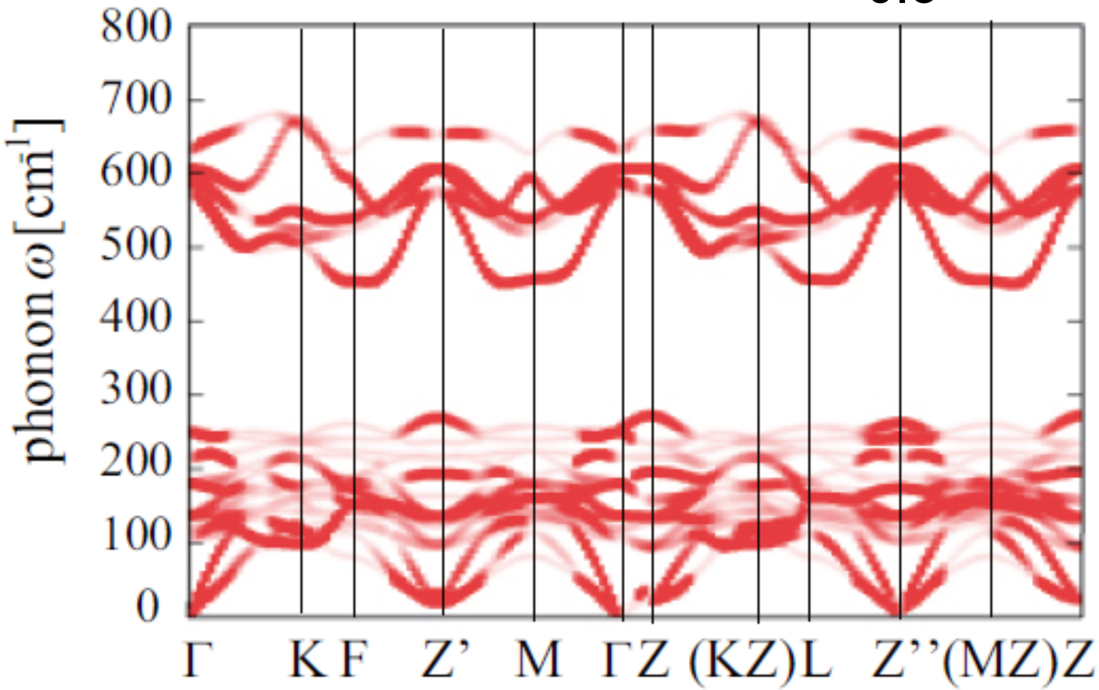
Result: calculation with F_{xc}^{ee}



T_c(SCDFT) < T_c(Exp)

Result: phonon spectrum & ele-ph coupling

$Li_{0.3}HfNCl$



Ele-ph coupling

$$\lambda = 2\int_0^{\infty} d\omega \frac{\alpha^2 F(\omega)}{\omega} = 0.83$$

Logarithmic averaged frequency

$$\omega_{\ln} = \exp\left(\frac{2}{\lambda}\int_0^{\infty} d\omega \frac{\alpha^2 F(\omega)}{\omega}\ln(\omega)\right)$$

$=324$ [cm^{-1}]

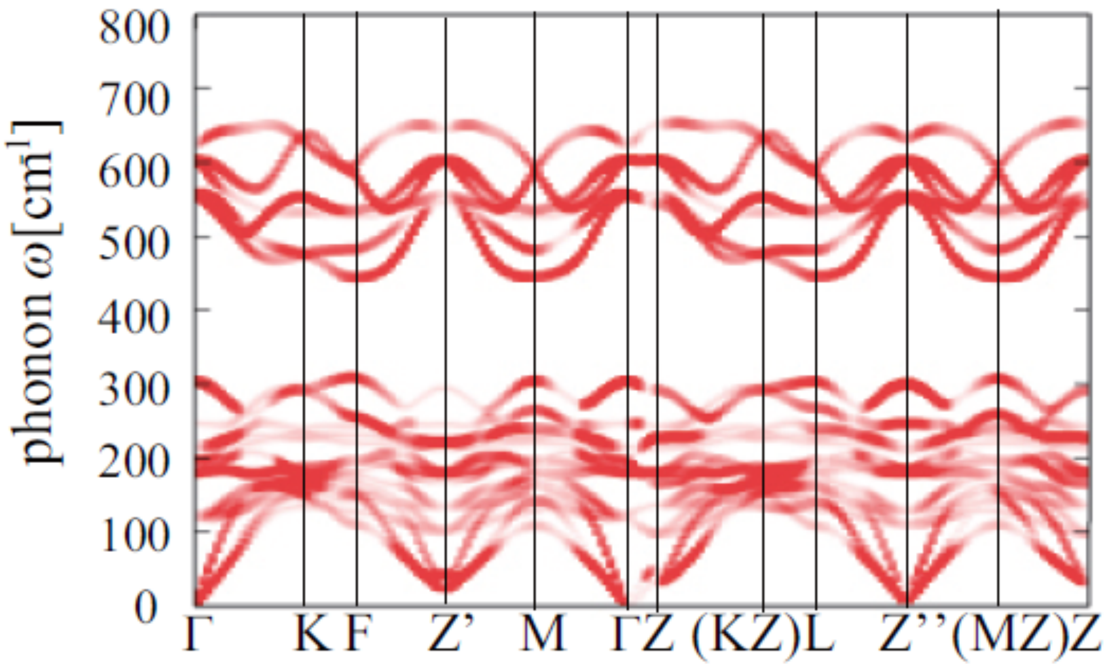
$$T_c = \frac{\omega_{\ln}}{1.2}\exp\left[-\frac{1.04(1+\lambda)}{\lambda}\right] = 27.1\mathrm{K}$$

$$\gamma_{q\lambda} = 2\pi\omega_{q\lambda}\sum_{k\nu\nu'} |g^{q\lambda}_{k+q\nu',k\nu}|^2 \delta(\epsilon_{k\nu})\delta(\epsilon_{k+q\nu'})$$

$$\alpha^2 F(\omega) = \frac{1}{2\pi N(E_F)}\sum_{q\lambda}\frac{\gamma_{q\lambda}}{\omega_{q\lambda}}\delta(\omega-\omega_{q\lambda})$$

Result: phonon spectrum & ele-ph coupling

$Li_{0.3}ZrNCl$



Ele-ph coupling

$$\lambda = 2\int_0^\infty d\omega \frac{\alpha^2 F(\omega)}{\omega} = 0.55$$

Logarithmic averaged frequency

$$\omega_{\ln} = \exp\left(\frac{2}{\lambda}\int_0^\infty d\omega \frac{\alpha^2 F(\omega)}{\omega}\ln(\omega)\right)$$

=420 [cm^{-1}]

$$T_c = \frac{\omega_{\ln}}{1.2}\exp\left[-\frac{1.04(1+\lambda)}{\lambda}\right] = 18.8\mathrm{K}$$

$$\gamma_{q\lambda} = 2\pi\omega_{q\lambda}\sum_{k\nu\nu'} |g^{q\lambda}_{k+q\nu',k\nu}|^2 \delta(\epsilon_{k\nu})\delta(\epsilon_{k+q\nu'})$$

$$\alpha^2 F(\omega) = \frac{1}{2\pi N(E_F)}\sum_{q\lambda}\frac{\gamma_{q\lambda}}{\omega_{q\lambda}}\delta(\omega-\omega_{q\lambda})$$

Raman active mode

[cm^{-1}]

Hf	
theory	Exp.
x=0.3	*x=0.35*
588	595
251	282
182	147
607	616
138	157
120	106

Result: x=0.3

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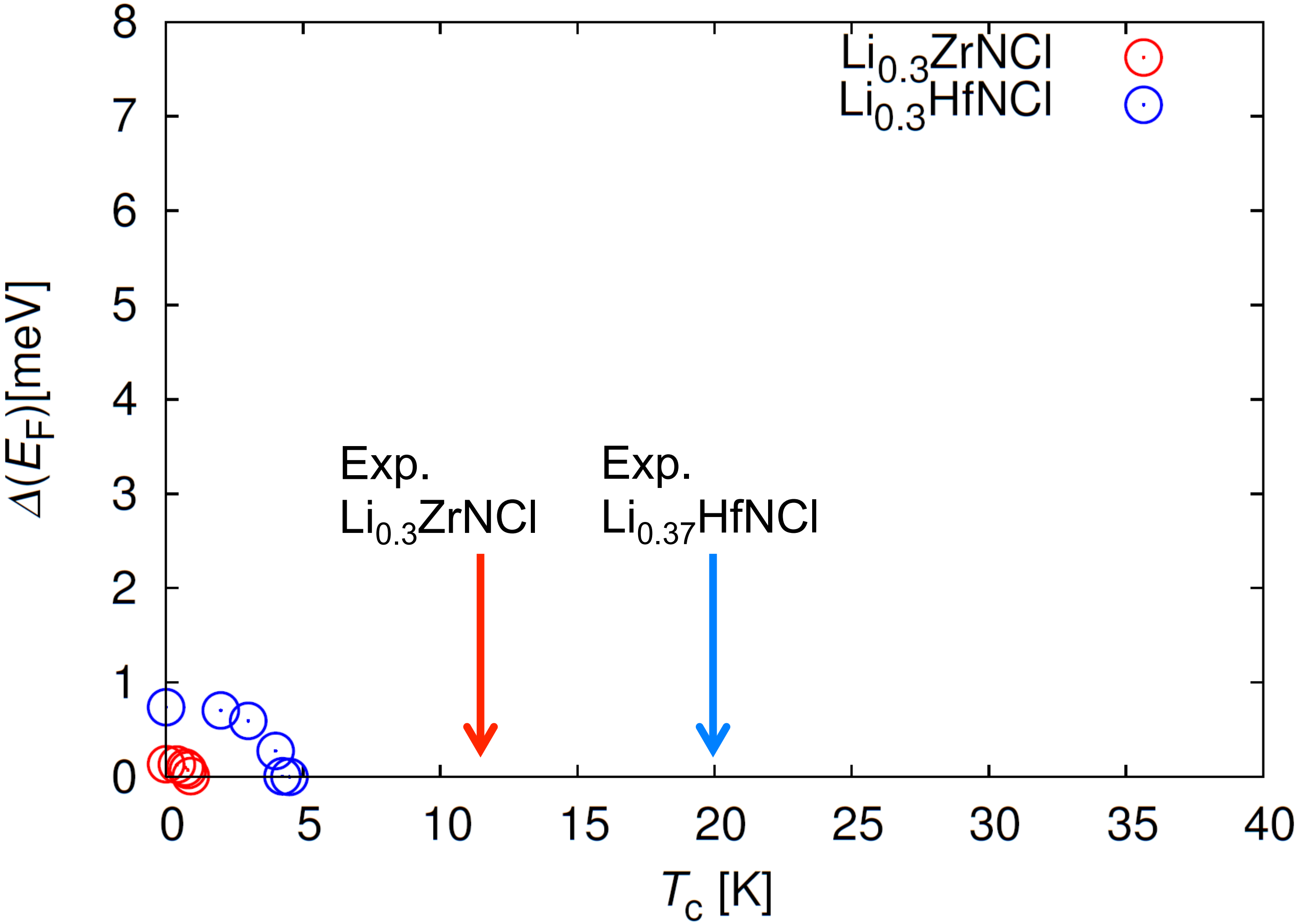
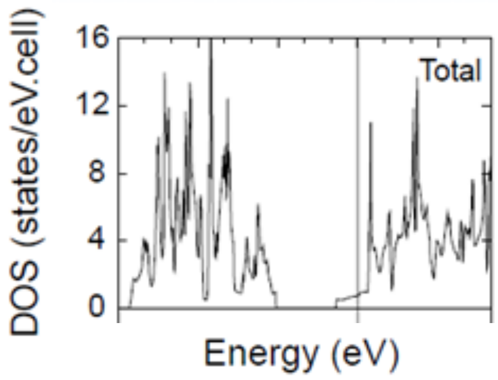


T_c(SCDFT) < T_c(Exp)

R.Arita

Discussion

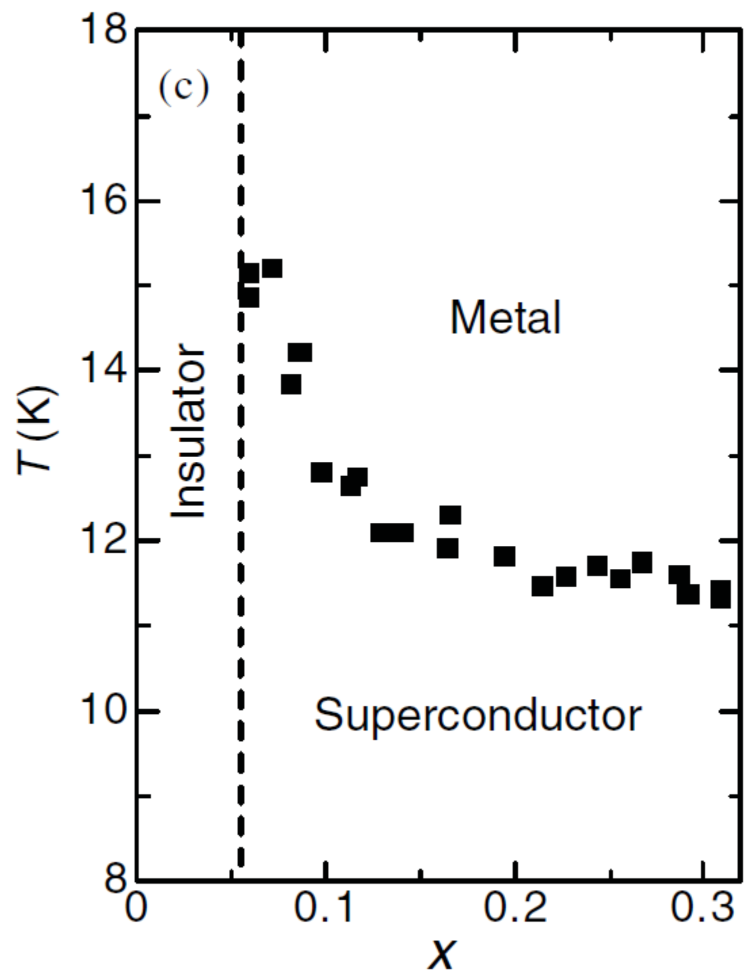


small x

small DOS

small λ

low T_c



Non Migdal-Eliashberg mechanism

Conclusion

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- Application of SC-DFT to layered nitride superconductors
  - T_c < 10K for x=0.3, 0.5
  - Unconventional superconductivity ?

- Construction of an exchange-correlation functional for unconventional superconductors