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Development of density functional theory for plasmon assisted superconductors

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In collaboration with
Ryosuke Akashi (Univ. Tokyo)

Poster 28 (arXiv:1303.5052, 1305.0390)

Poster 29 (arXiv:1303.5138)
SCDFT study on Alkali-doped fullerides

Yusuke Nomura (Univ. Tokyo)

Poster 26 (arXiv:1305.2995)
Ab initio downfolding method for electron-phonon coupled systems & Application to iron-based superconductors

Outline

Lecture by Prof. Profeta
Gross et al., 1988, 2001, 2005

- DFT for superconductors (SCDFT)
  - Formalism free from empirical parameters (such as μ^* in the Migdal-Eliashberg theory)
  - T_c reproduced successfully for conventional superconductors (such as simple metals, MgB_2, CaC_6…)
- Development of SCDFT for unconventional SC
  - Plasmon mechanism
  - Application to Li under high pressure (T_c >10K)

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

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

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

(Nuclei are treated by the Born-Oppenheimer approx.)

DFT for superconductors

Oliveira et al., PRL 60, 2430 (1988)
Kreibich & Gross PRL 86, 2984 (2001)
M. Lüders et al, PRB 72, 024545 (2005)
M. Marques et al, PRB 72, 024546 (2005)

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

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

Oliveira et al., PRL 60, 2430 (1988)
Kreibich & Gross PRL 86, 2984 (2001)
M. Lüders et al, PRB 72, 024545 (2005)
M. Marques et al, PRB 72, 024546 (2005)

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

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

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

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

Gap equation

Oliveira et al., PRL 60, 2430 (1988)
Kreibich & Gross PRL 86, 2984 (2001)
M. Lüders et al, PRB 72, 024545 (2005)
M. Marques et al, PRB 72, 024546 (2005)

Linearized gap equation

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

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

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

Once F_{xc} is given, we can calculate T_c without adjustable parameters

Migdal-Eliashberg Theory

Self-consistent perturbation theory:
lowest-order dressed-phonon and dressed Coulomb contribution to Σ retained

(Nambu-Gor'kov formalism)

$$\overline{\Sigma}(\mathbf{k}, i\omega_n) = -k_B T \sum_{\mathbf{k}', n'} \overline{\tau_3} \overline{G}(\mathbf{k}', i\omega_{n'}) \overline{\tau_3} \left[\sum_{\lambda} \left\{ g_{\mathbf{k}\mathbf{k}'\lambda} \right\}^2 D_\lambda(\mathbf{k}-\mathbf{k}', i\omega_n - i\omega_{n'}) + V_c(\mathbf{k}-\mathbf{k}') \right] \frac{d^4 p'}{(2\pi)^4}$$

Damping and retardation effects are considered

Can we take account of these effects in the framework of DFT ?

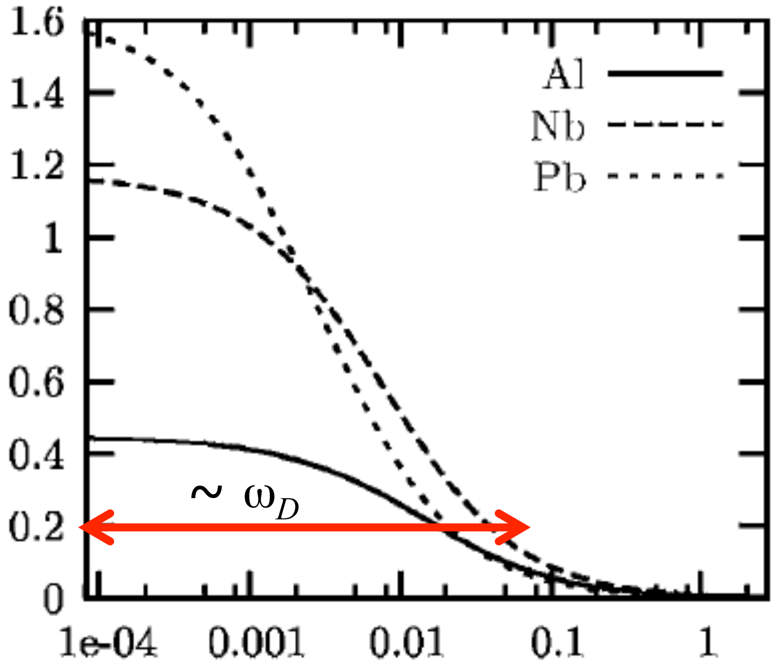
In DFT, everything is represented in terms of density …

Retardation effect in SCDFT

Gap equation in SCDFT→ No ω dependence, but state dependent

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

Almost state independent

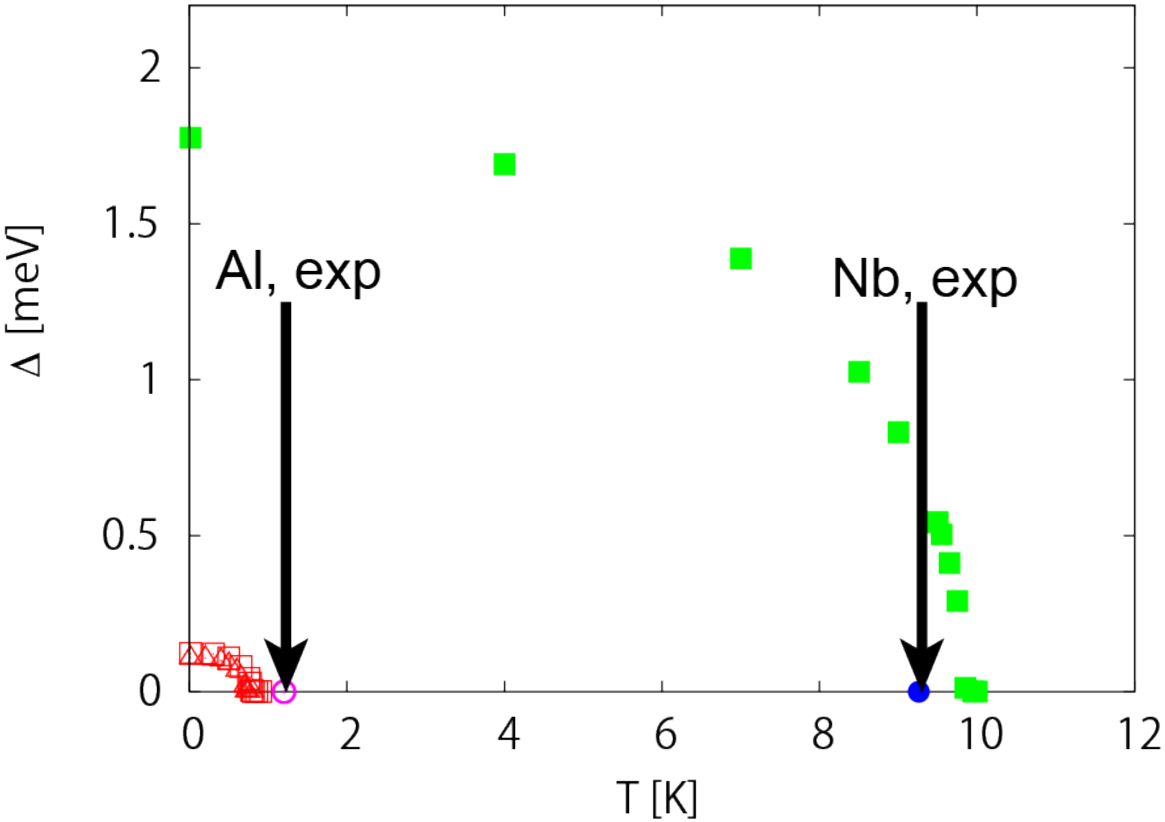


Kohn-Sham energy ξ of ϕ_i [eV]

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

Application to simple metals

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



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

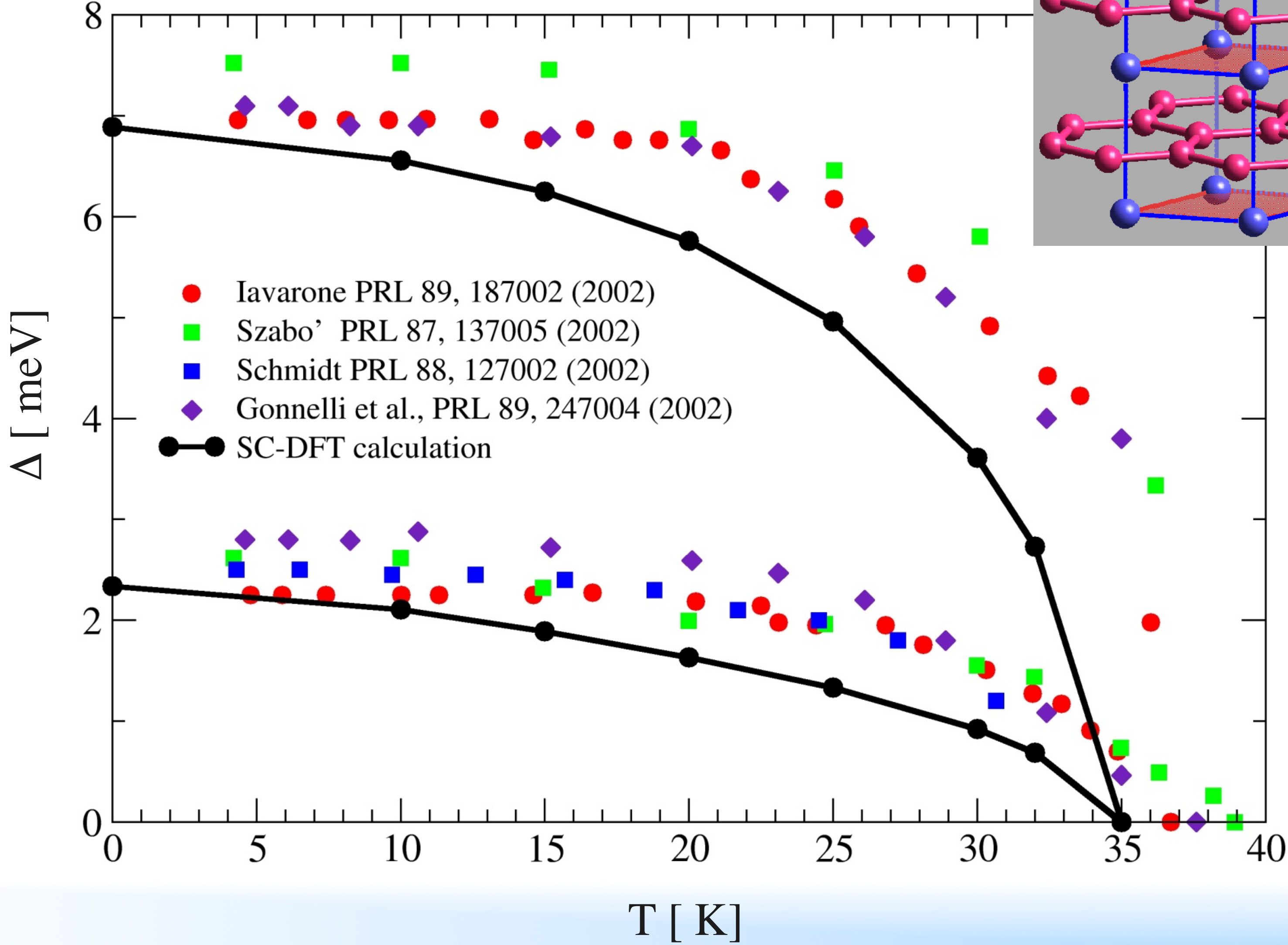
	Al	Nb	Ta	Pb	Cu
DFT	0.9	9.5	3.7	6.9	<0.01
Experimental	1.18	9.5	4.5	7.2	-

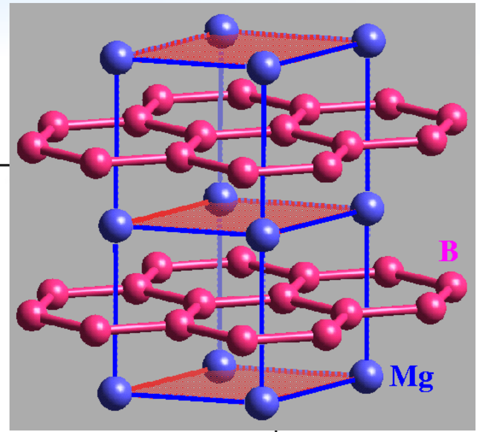
Gap at zero temperature

	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

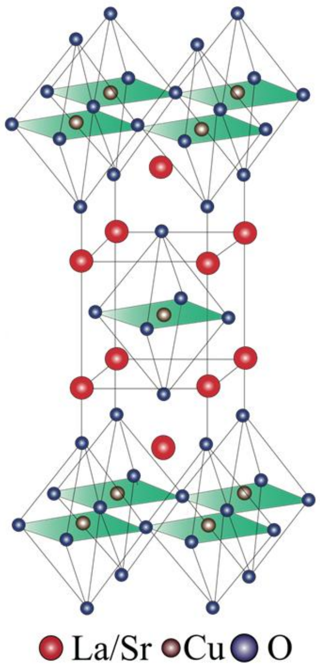
A. Floris et al, Phys. Rev. Lett. 94, 037004 (2005)

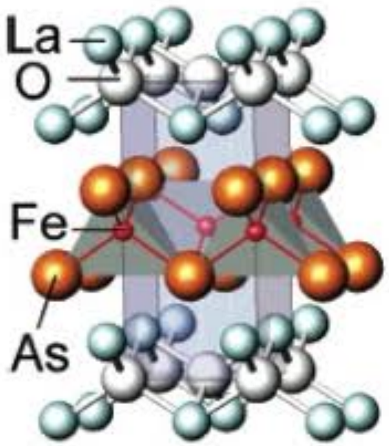


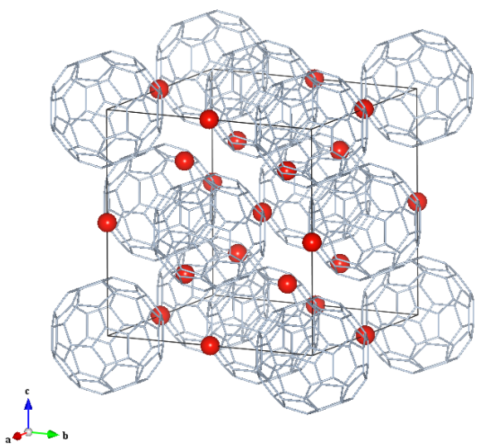


Application to unconventional SC

$La_{2-x}Sr_xCuO_4$





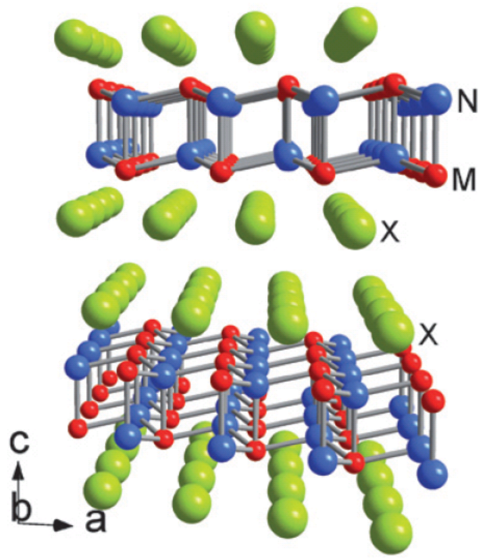


R. Akashi and RA, arXiv:1303.5152

MNX

M=Zr, Hf

X= Cl, Br, I



R. Akashi, K. Nakamura, RA and M. Imada PRB2012

DFT for unconventional SC

It is an interesting challenge to formulate DFT for unconventional SC

- spin-fluctuation mediated SC
- orbital-fluctuation mediated SC
- exciton mechanism
- → plasmon mechanism

…

Plasmon mechanism

Proposed by Y. Takada JPSJ 45 786 (1978)

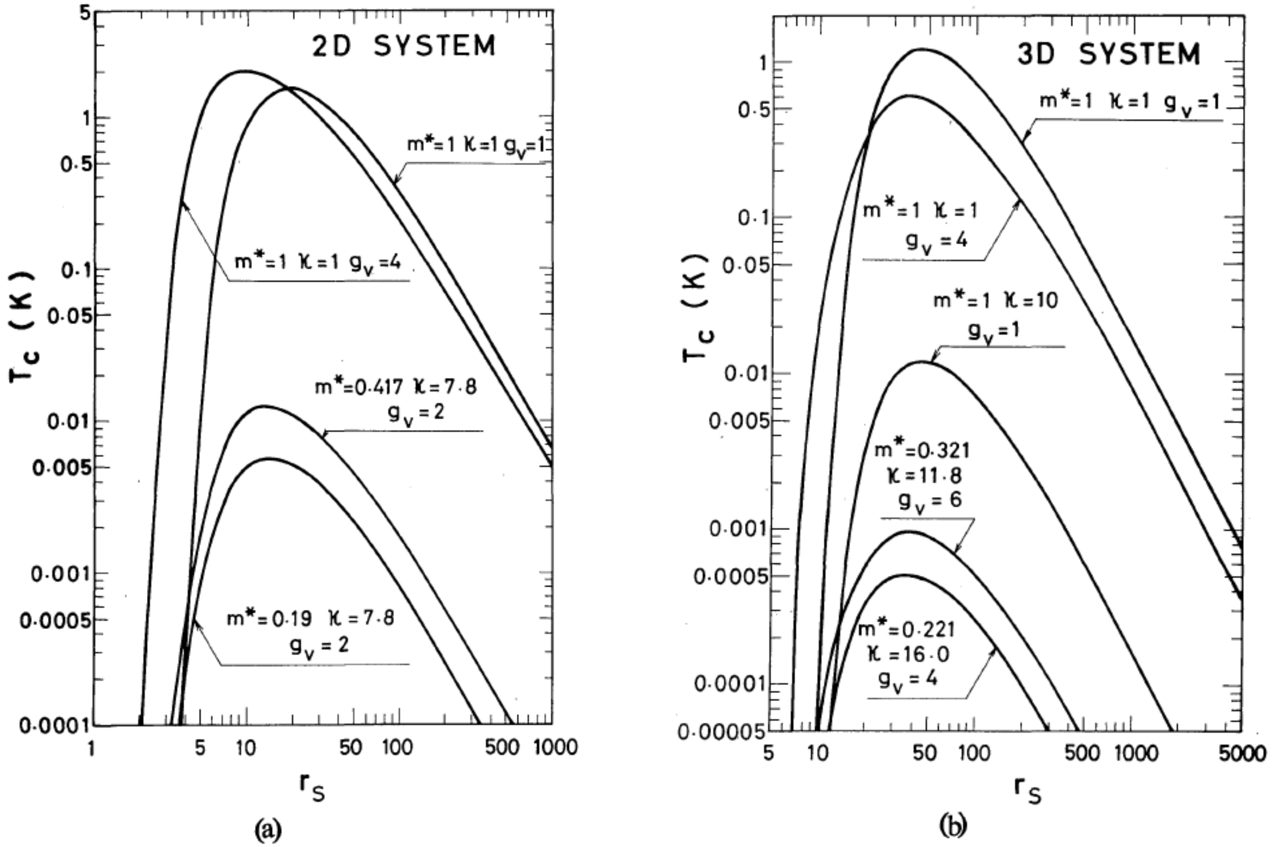


Fig. 2. Calculated results of T_c for several values of m^*, κ, and g_v. A 2D system is treated in (a), while a 3D one is in (b).

Superconducting ground state for large r_s

Plasmon mechanism

$SrTiO_3$
Y. Takada JPSJ 49 1267 (1980)

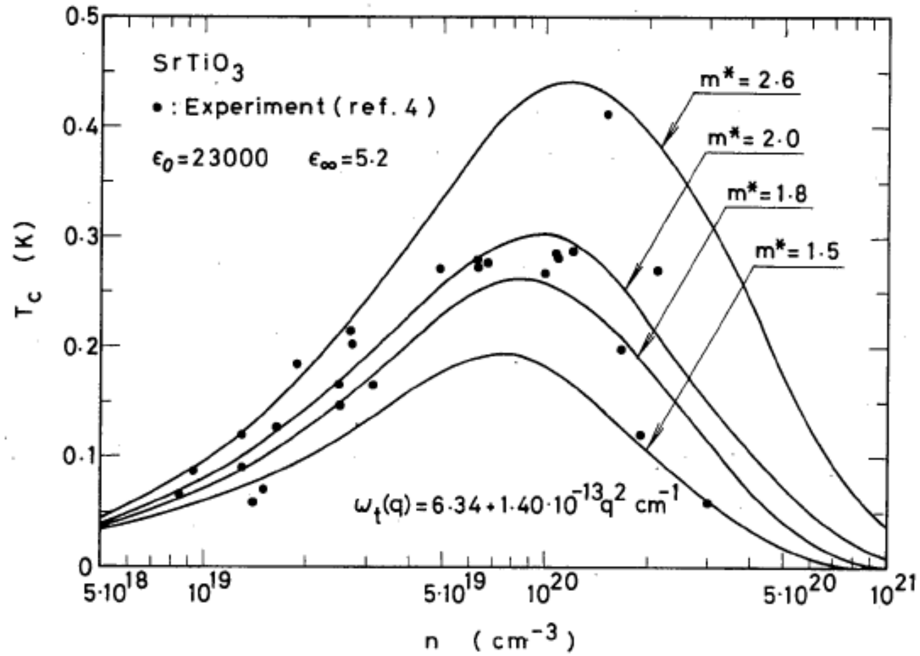
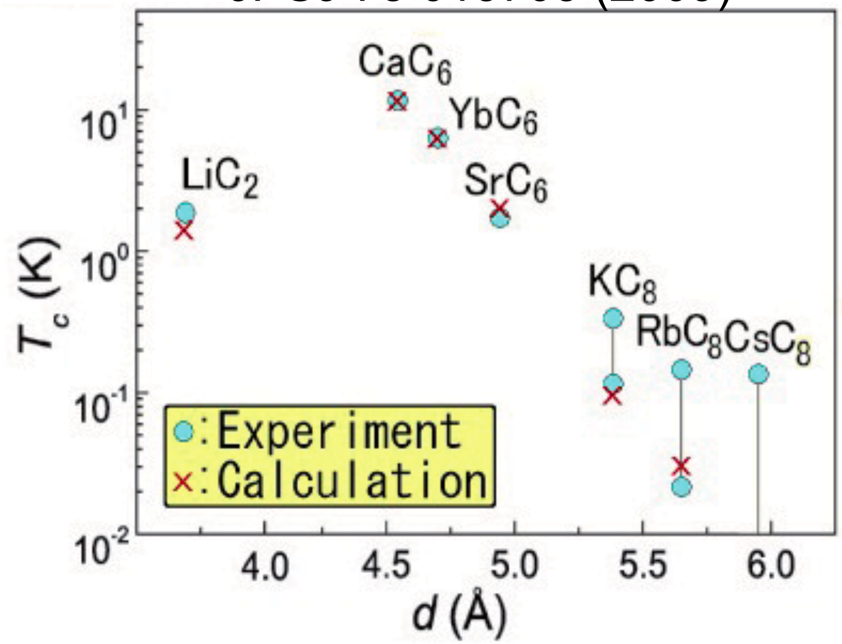


Fig. 6. Calculated T_c as a function of n for several values of m^* in the plasmon-FE soft phonon mechanism of superconductivity.

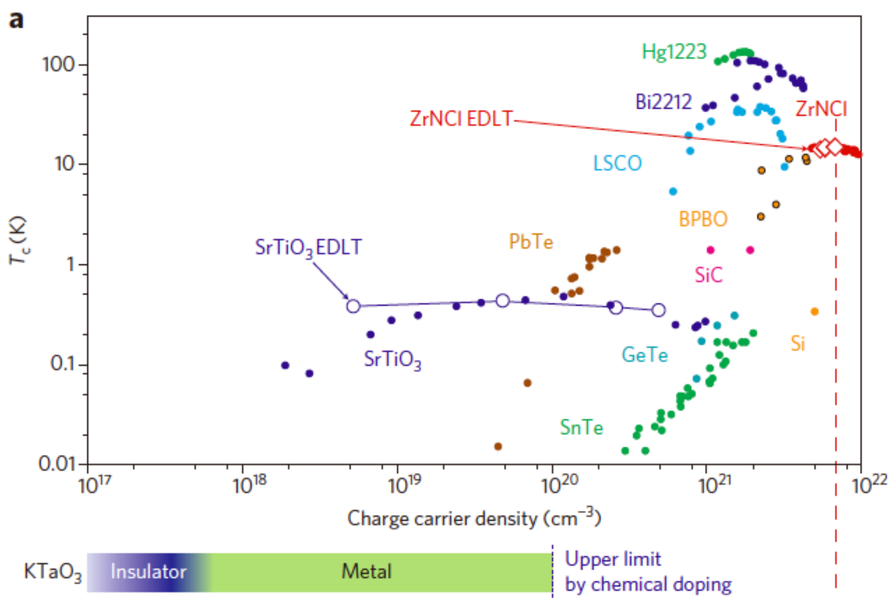
GIC
Y. Takada JPSJ 51 63 (1982), JPSJ 78 013703 (2009)

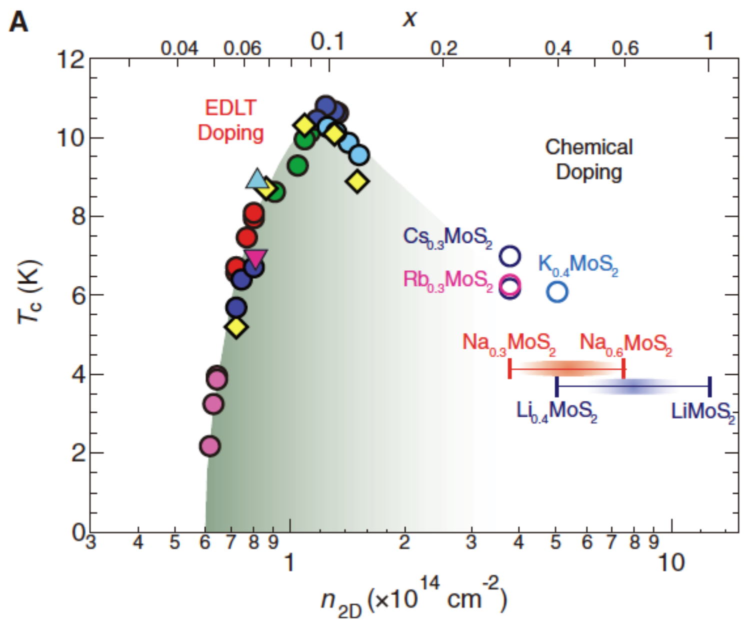


Cooperation of phonon & plasmon enhances pairing instability

SC in doped insulators

Field-induced SC has been observed in a variety of band insulators





K. Ueno et al.,
Nature Nanotechnology 6 408 (2011)

J.T. Ye et al.,
Science 338 1193 (2012)

Tc has a dope-like shape
Peak in low density region

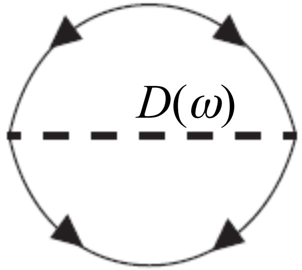
How to describe the plasmon mechanism in DFT

$$\Delta_i = \frac{-1}{2}\sum_j K_{ij}^{\mathrm{Hxc}} \frac{\tanh[\beta\xi_j/2]}{\xi_j}\Delta_j \qquad K_{ij}^{\mathrm{Hxc}} = \frac{\delta^2(E_H + F_{xc})}{\delta\chi_i^*\delta\chi_j}$$

Kohn-Sham perturbation theory (F, D, V_c are obtained from first-principles calc.)

F (anomalous Green fn.)

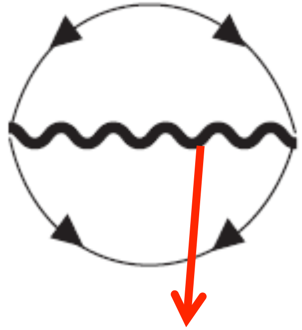
$F_{xc}^{e\text{-}ph} =$



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

F (anomalous Green fn.)

$F_{xc}^{e\text{-}e} =$



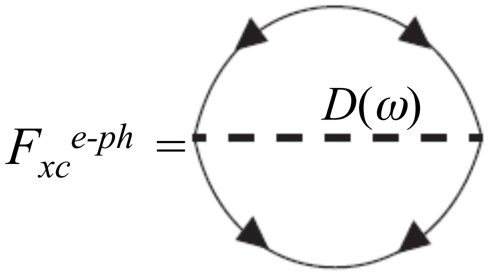
Static screened Coulomb V_c

How to describe the plasmon mechanism in DFT

$$\Delta_i = \frac{-1}{2} \sum_j K_{ij}^{\mathrm{Hxc}} \frac{\tanh[\beta \xi_j / 2]}{\xi_j} \Delta_j \qquad K_{ij}^{\mathrm{Hxc}} = \frac{\delta^2 (E_H + F_{xc})}{\delta \chi_i^* \delta \chi_j}$$

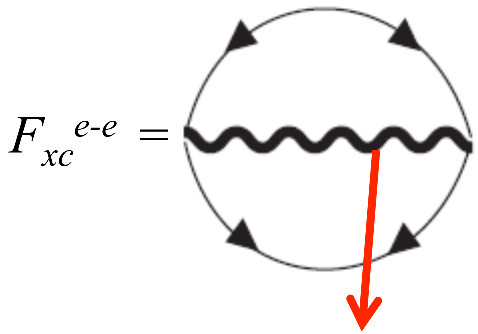
Kohn-Sham perturbation theory (F, D, V_c are obtained from first-principles calc.)

F (anomalous Green fn.)



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

F (anomalous Green fn.)



Dynamical screened Coulomb $V_c(\omega)$
with plasmon-pole approximation

How to describe the plasmon mechanism in DFT

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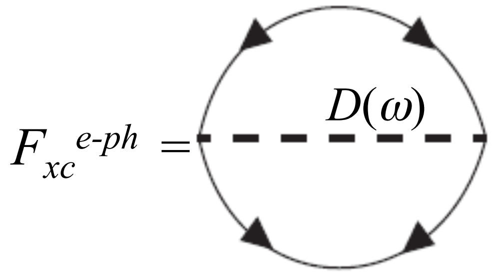
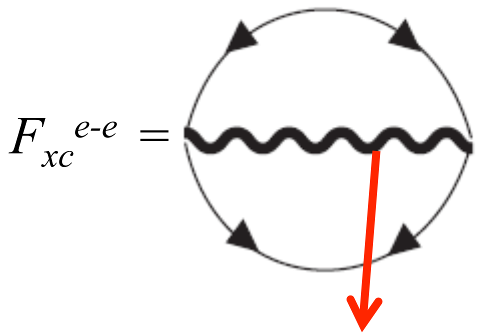
Kohn-Sham perturbation theory (F, D, V_c are obtained from first-principles calc.)

F (anomalous Green fn.)



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

F (anomalous Green fn.)



Dynamical screened Coulomb $V_c(\omega)$
with plasmon-pole approximation

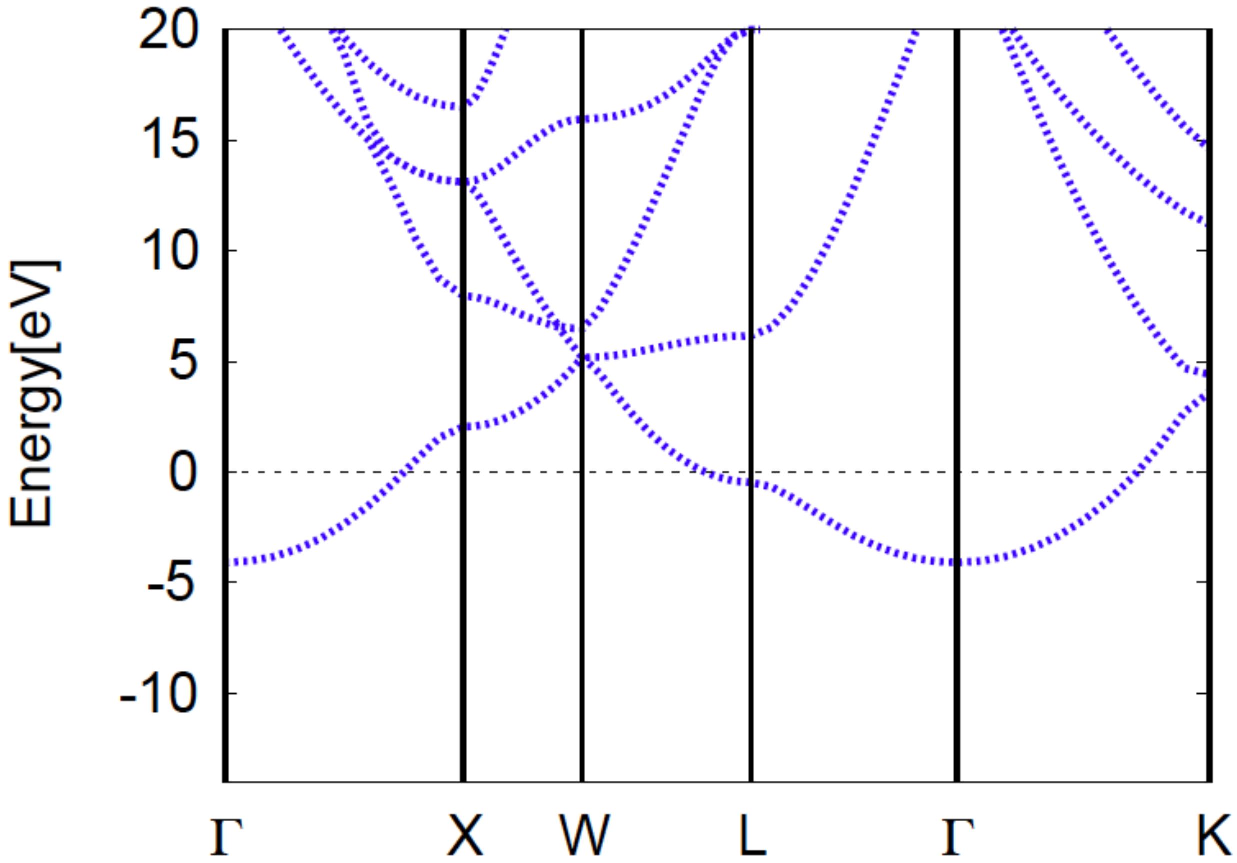
$$\mathcal{K}^{\mathrm{el,dyn}}_{n\mathbf{k},n'\mathbf{k}'} = \frac{1}{\tanh[(\beta/2)E_{n\mathbf{k}}]}\frac{1}{\tanh(\beta E_{n'\mathbf{k}'}/2)}\frac{1}{\beta^2} \times \sum_{\omega_1\omega_2} F_{n\mathbf{k}}(\mathrm{i}\omega_1)F_{n\mathbf{k}}(\mathrm{i}\omega_2)W_{n\mathbf{k}n'\mathbf{k}'}[\mathrm{i}(\omega_1-\omega_2)]$$

$$\tilde{W}_{n\mathbf{k}n'\mathbf{k}'}(\mathrm{i}\omega_m) = W_{n\mathbf{k}n'\mathbf{k}'}(0) + \sum_i^{N_p} a_{i;n\mathbf{k}n'\mathbf{k}'}\left[\frac{2}{\omega_{i;n\mathbf{k}n'\mathbf{k}'}} - \frac{2\omega_{i;n\mathbf{k}n'\mathbf{k}'}}{\omega_m^2 + \omega^2_{i;n\mathbf{k}n'\mathbf{k}'}}\right]$$

$$F_{n\mathbf{k}}(\mathrm{i}\omega) = \frac{1}{\mathrm{i}\omega + E_{n\mathbf{k}}} - \frac{1}{\mathrm{i}\omega - E_{n\mathbf{k}}}$$

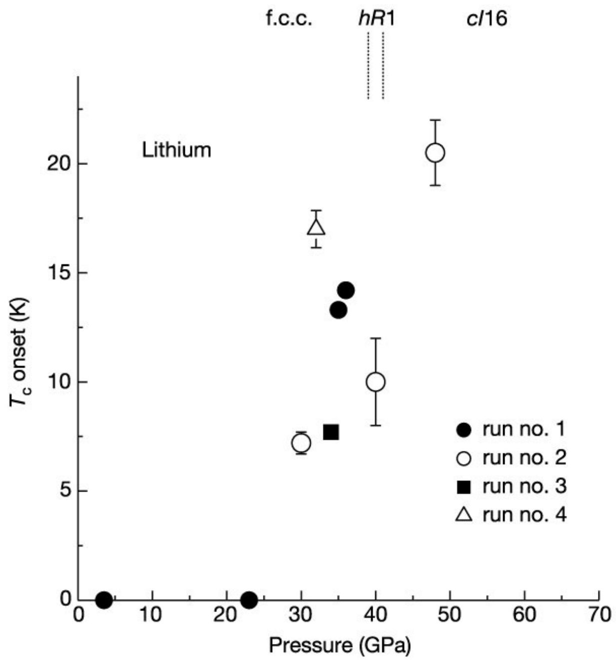
R.Arita

Li: band structure

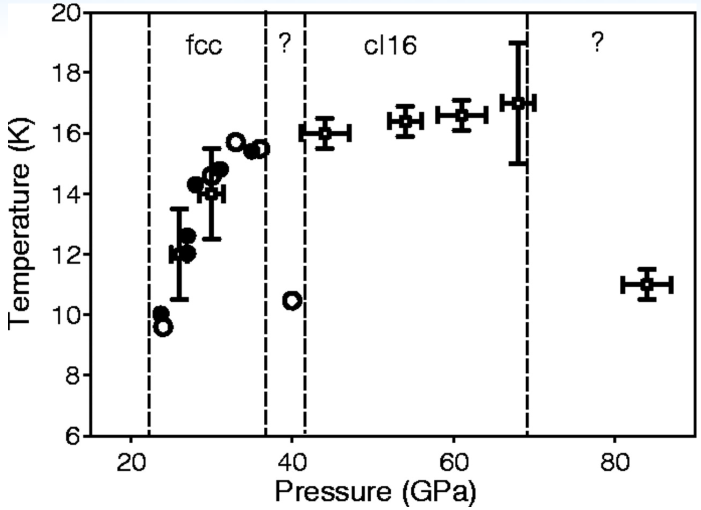


Band structure ~ Nearly Free Electron (NFE) model

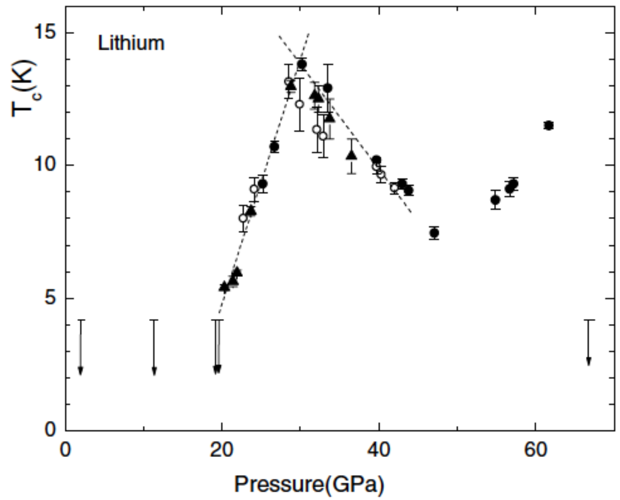
High T_c SC in Li under high pressure: experiments



Shimizu et al., Nature 419, 597 (2002)
T_c~20K at 48GPa

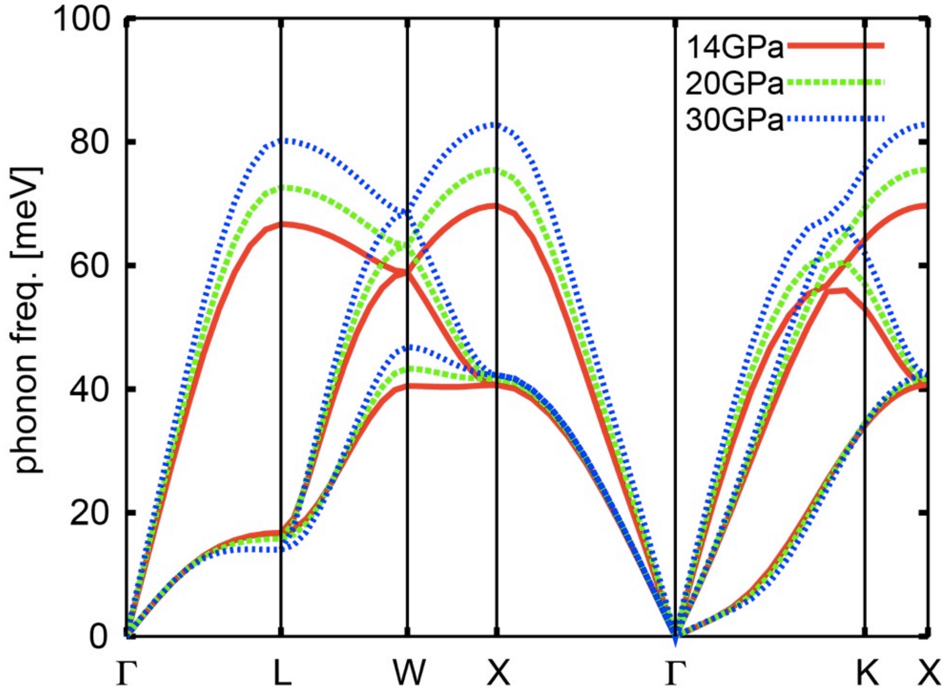


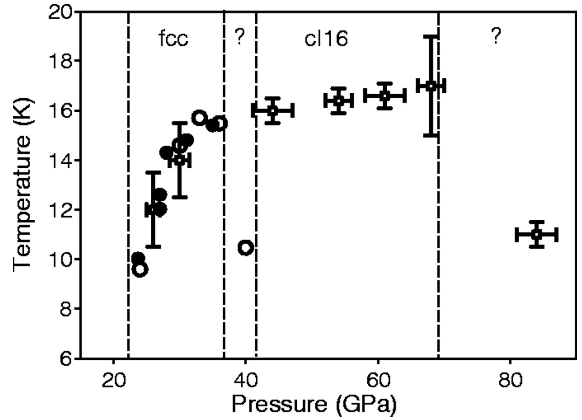
Struzhkin et al., Science 298, 1213 (2002)



Deemyad and Schilling, PRL 91, 167001 (2003)

Li under high pressure: conventional scenario ?

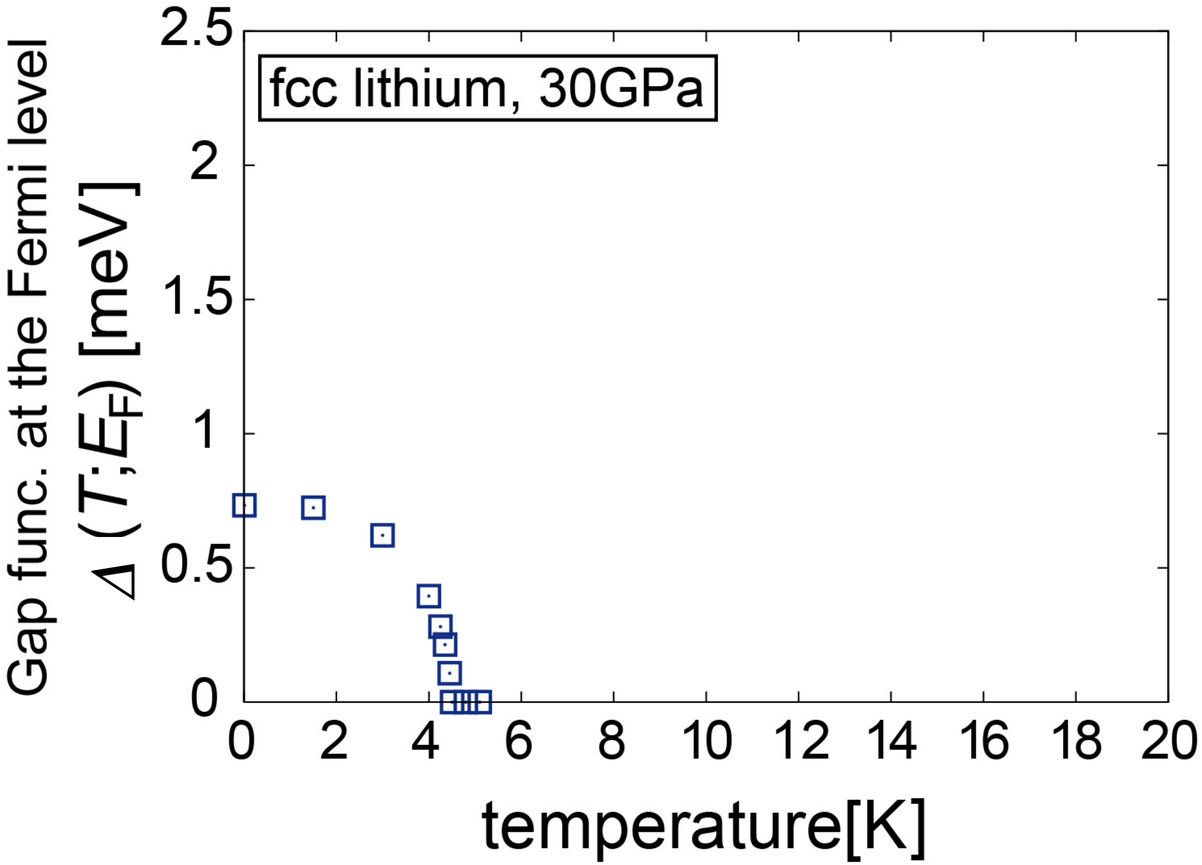




Pressure [GPa]	14	20	30
Ele-ph coupling (λ)	0.522	0.623	0.812

Consistent with T. Bazirov et al., PRB 82, 184509 (2010)

Conventional SCDFT calc. for Li



High T_c SC in Li under high pressure: experiments

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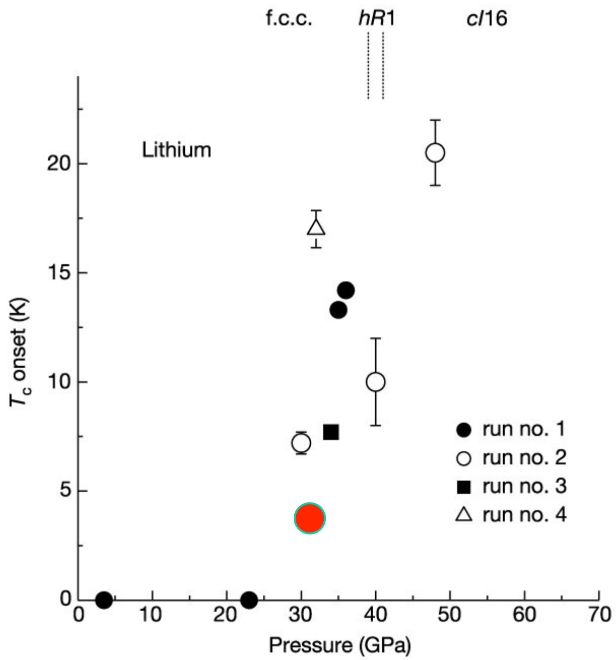
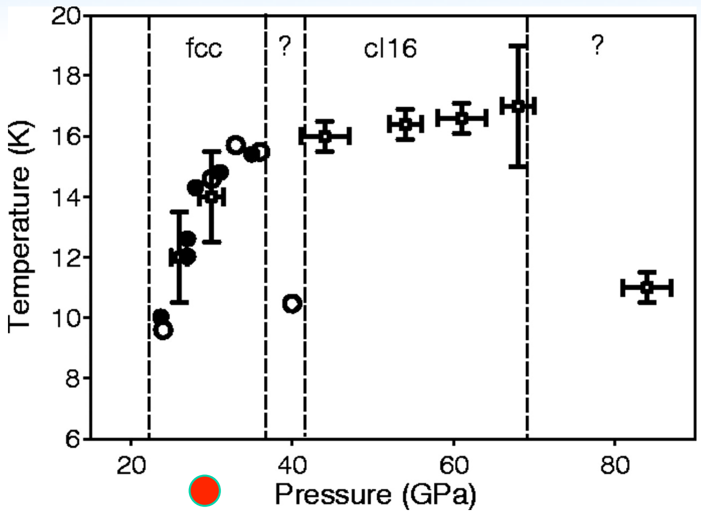
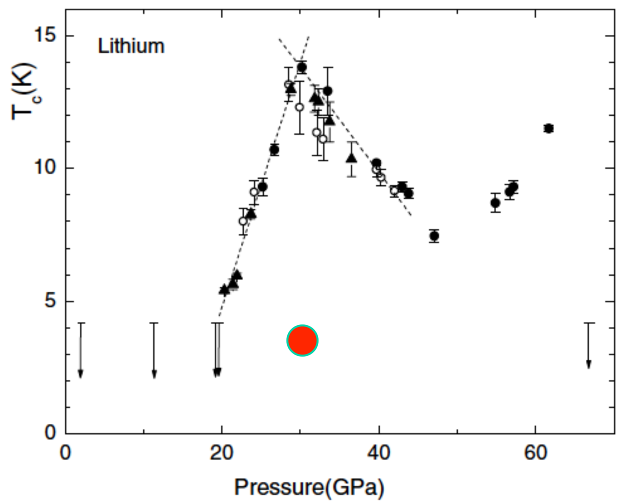


Shimizu et al., Nature 419, 597 (2002)
T_c~20K at 48GPa
(highest T_c of any elements)

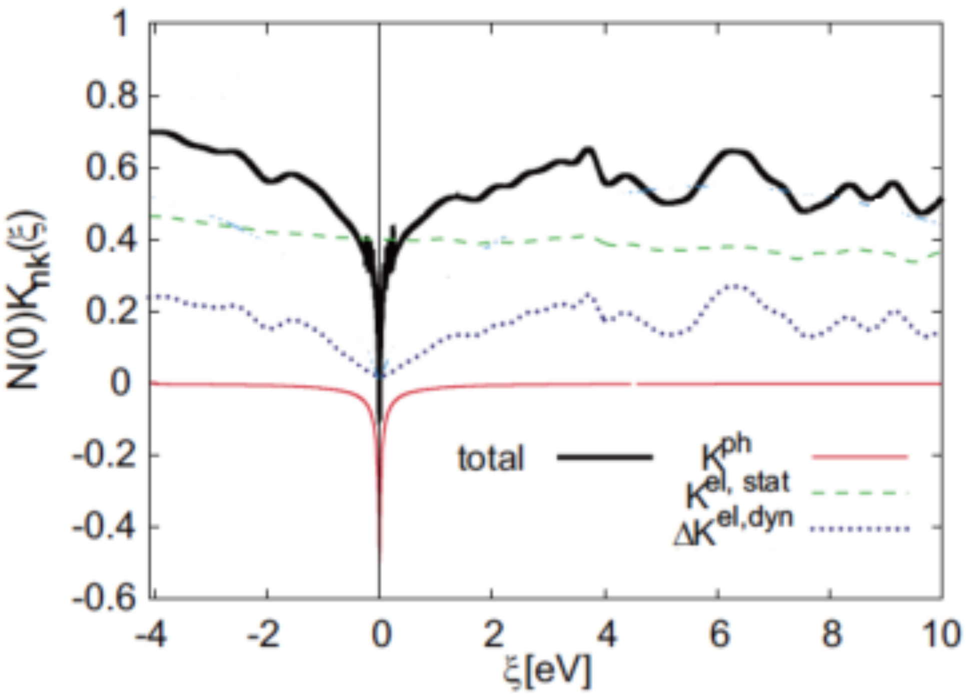


Struzhkin et al., Science 298, 1213 (2002)



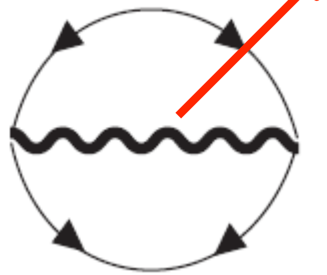
Deemyad and Schilling, PRL 91, 167001 (2003)

Application to Li: Exch-Corr. Kernel



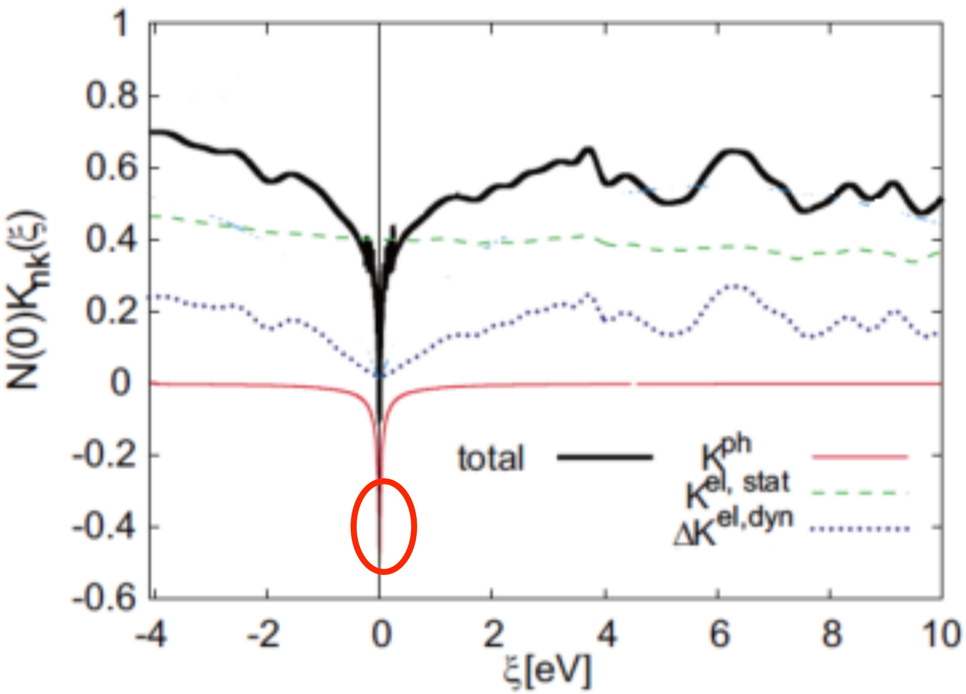
Dynamical screened Coulomb $V_c(\omega)$

$F_{xc}^{e\text{-}e} =$



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

Application to Li: Exch-Corr. Kernel



Dynamical screened Coulomb $V_c(\omega)$

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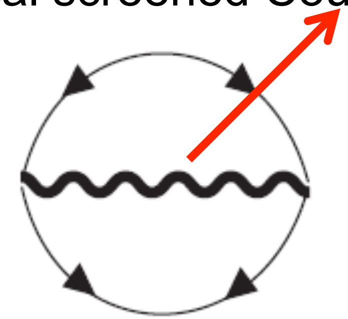
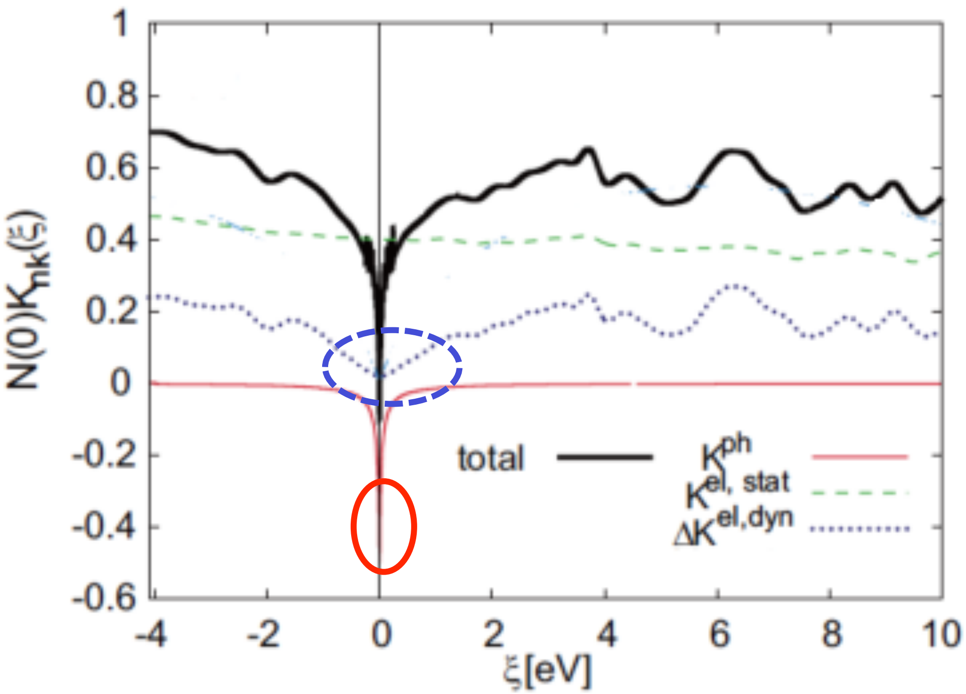


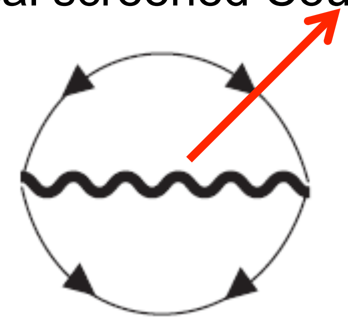
$$K_{ij}^{\mathrm{Hxc}} = \frac{\delta^2 (E_H + F_{xc})}{\delta\chi_i^* \delta\chi_j}$$

Application to Li: Exch-Corr. Kernel



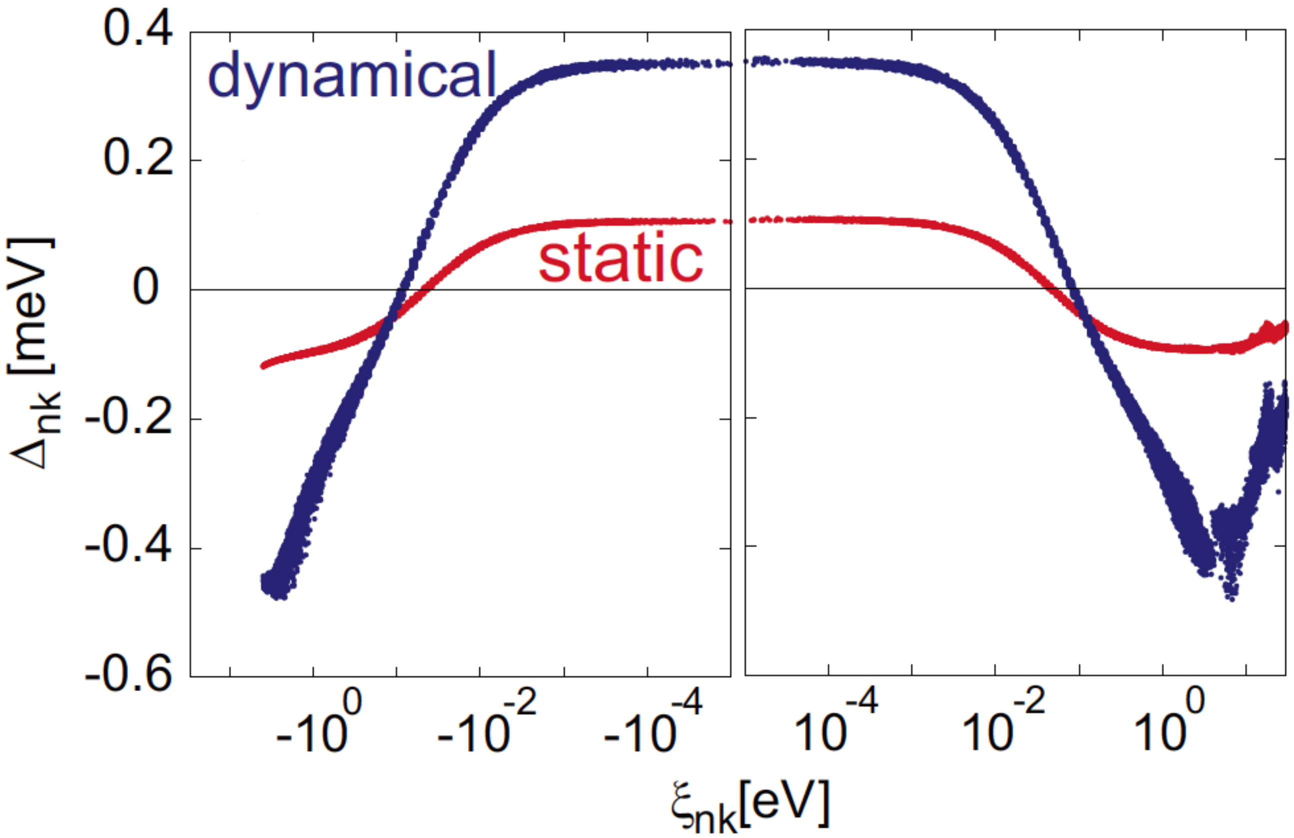
Dynamical screened Coulomb $V_c(\omega)$

$F_{xc}^{e\text{-}e} =$

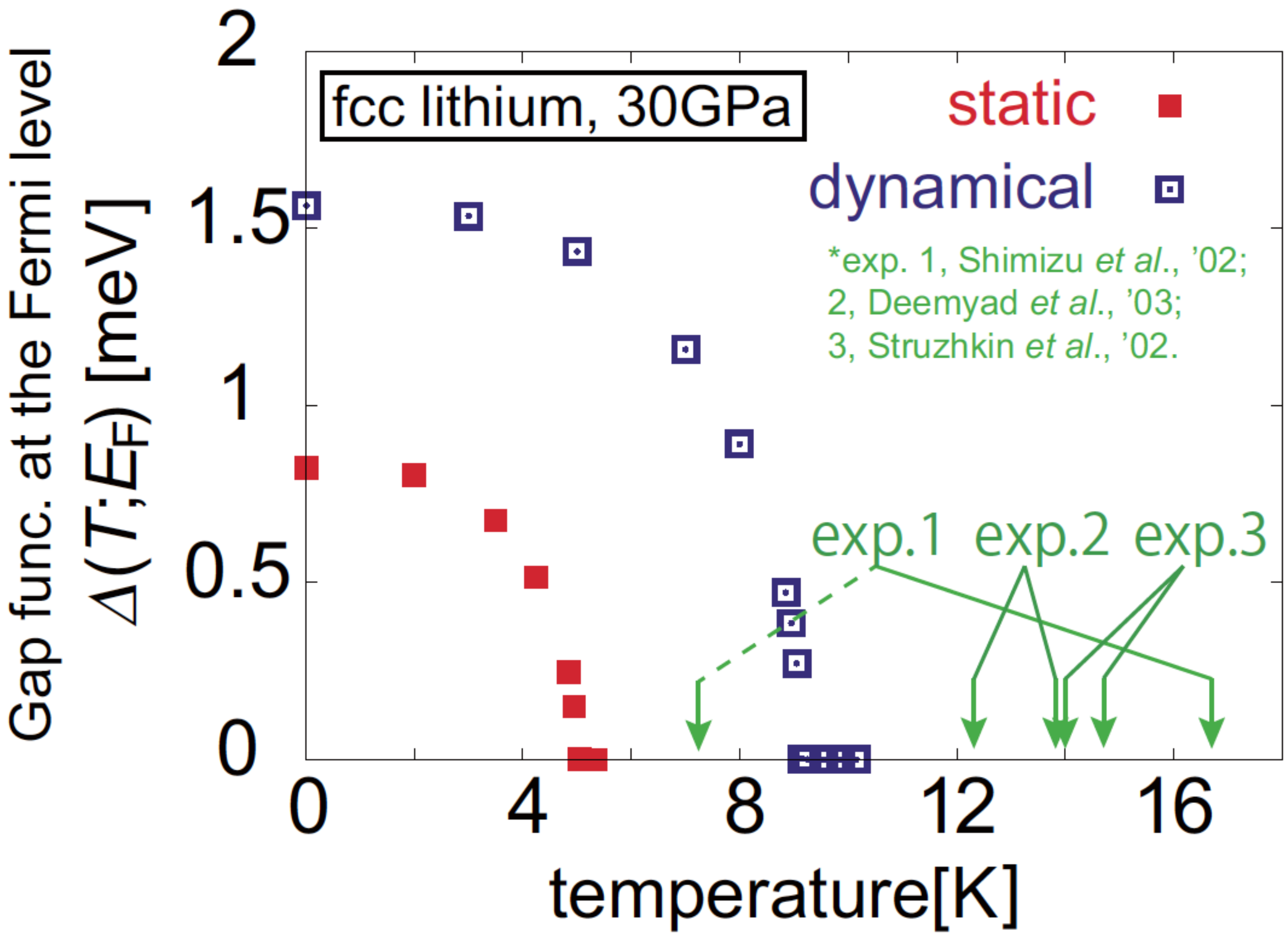


$$K_{ij}^{\mathrm{Hxc}} = \frac{\delta^2 (E_H + F_{xc})}{\delta\chi_i^* \delta\chi_j}$$

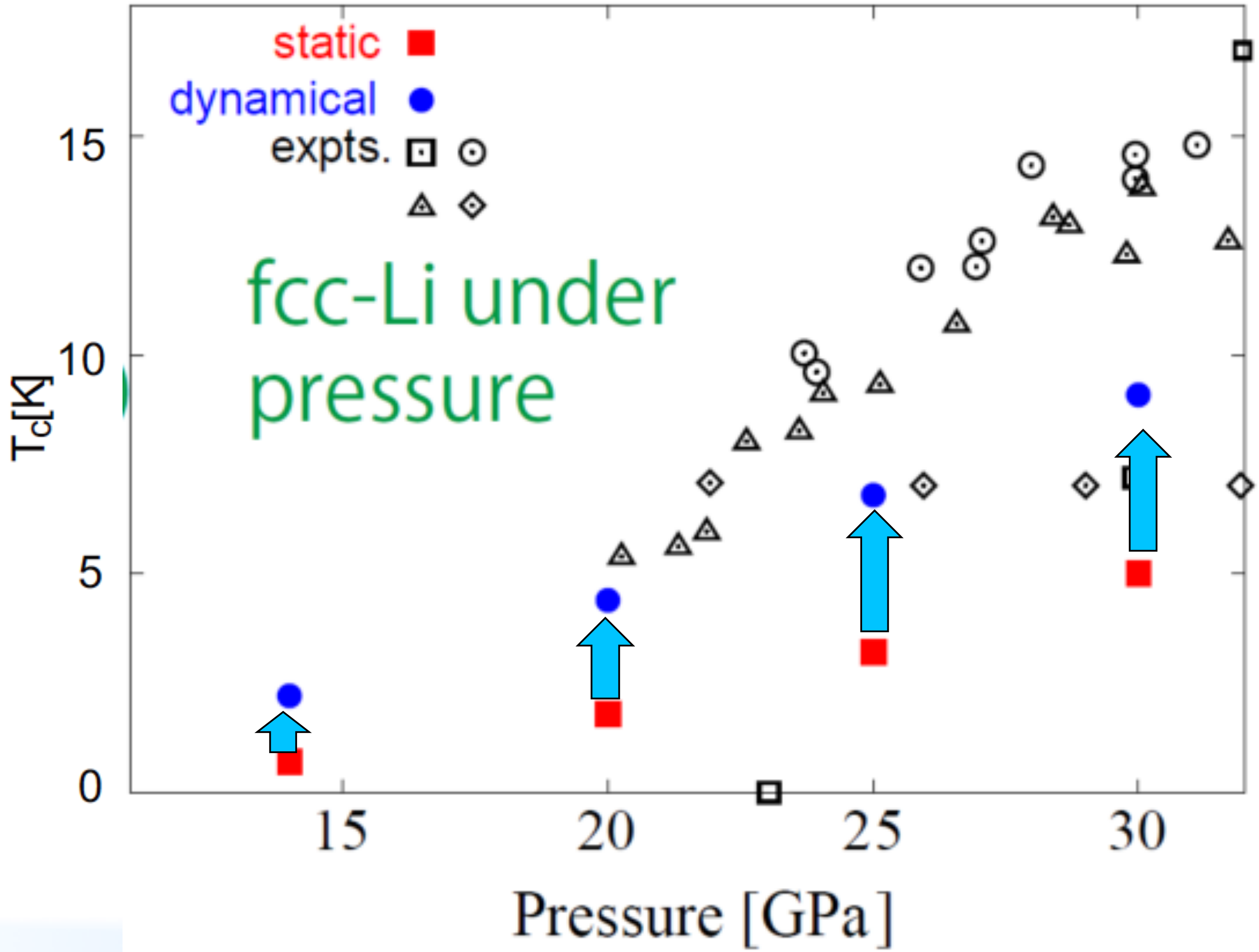
Application to Li: Gap function at T=0



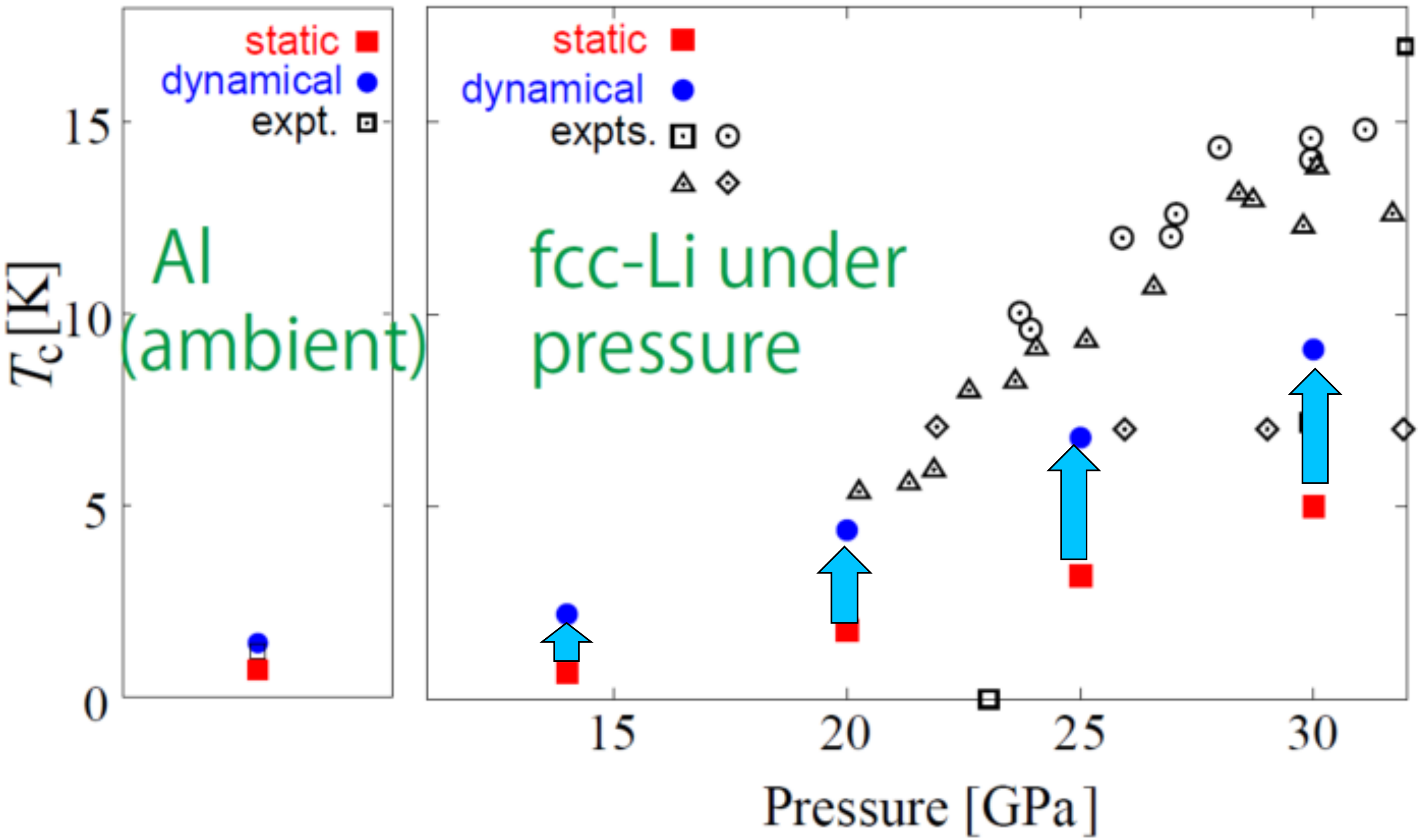
Application to Li: Gap function



Application to Li: T_c



Application to Al: T_c



Summary & Outlook

- Development of SCDFT for unconventional SC
  - Plasmon assisted SC
  - Application to Li under high pressure

- Application to other systems such as MoS_2, HfNCl, …
- Development of SCDFT for other mechanisms
  - Spin fluctuation mediated SC
  - …