Electron-phonon coupling from optics

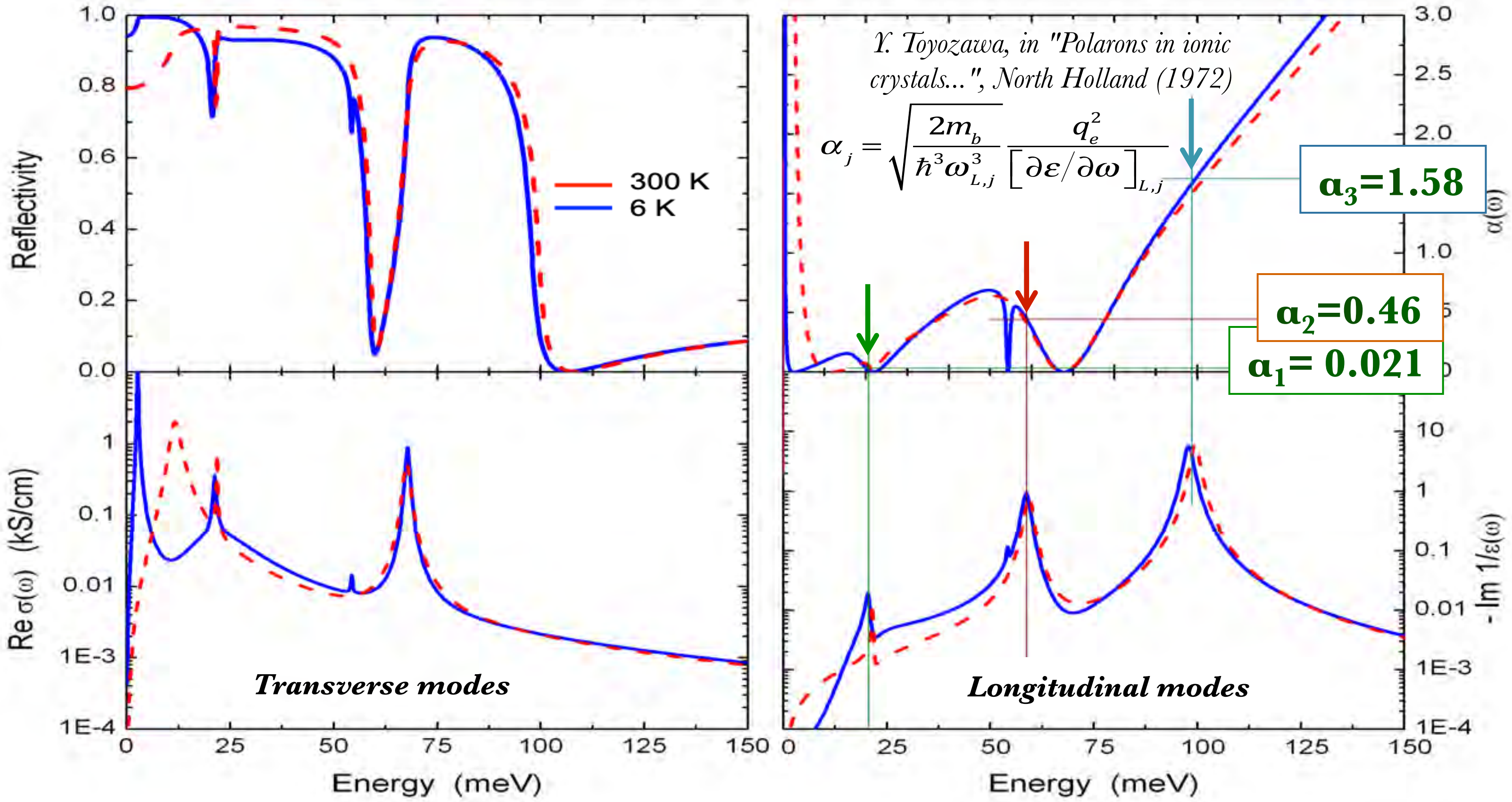
Dirk van der Marel*

I. Ardizzone*[10], N.P. Armitage*[1], F. Barantani*[11], F. Baumberger£[2], C. Barreteau*[7], C. Berthod*[9], M. Boselli*[10], C.-C. Chen$[2], J.T. Devreese♭[3,5,6,8], T.P. Devereaux$[2], A. Fête*[9], S.-I. Fujimori§[2], S. Gariglio*[9.10], E. Giannini*[7,12], C. Grimaldi*[1], H. Hagemann*[1], R.H. He$[2], D. Jaccard*[7], S.N. Klimin♭[3,5,6,8], A.B. Kuzmenko*[1,10], D.H. Lu$[2], W. Luo*[10], I.I. Mazin♮[1,4], J.L.M.van Mechelen*[1,3,4], W. Meevasana$[2], S.-K. Mo$[2], R.G. Moore$[2], B. Moritz$[2], N. Nagaosa¶[2], D. Pullmannova*[12], J.-M. Poumirol*[7,10], Z. Ren*[7], N. Reyren*[1], C.W. Rischau*[11,12], G. Scheerer*[7,12], A. Stucky*[7], Tempere♭[5,6,8], J. Teyssier*[10], Z.-X. Shen$[2], J.-M. Triscone*[9,10], D. Valentinis*[9], X.J. Zhou¥[2], J. Zaanen€[2]

*Université de Genève, Switzerland
£University of St Andrews, UK
$Stanford University, USA
♭ Universiteit Antwerpen, Belgium
♮Naval Research Laboratory, Washington DC, USA
¥Chinese Academy of Sciences, Beijing, China
§Japan Atomic Energy Agency, Mikazuki, Japan
¶The University of Tokyo, Japan
€Leiden University, The Netherlands

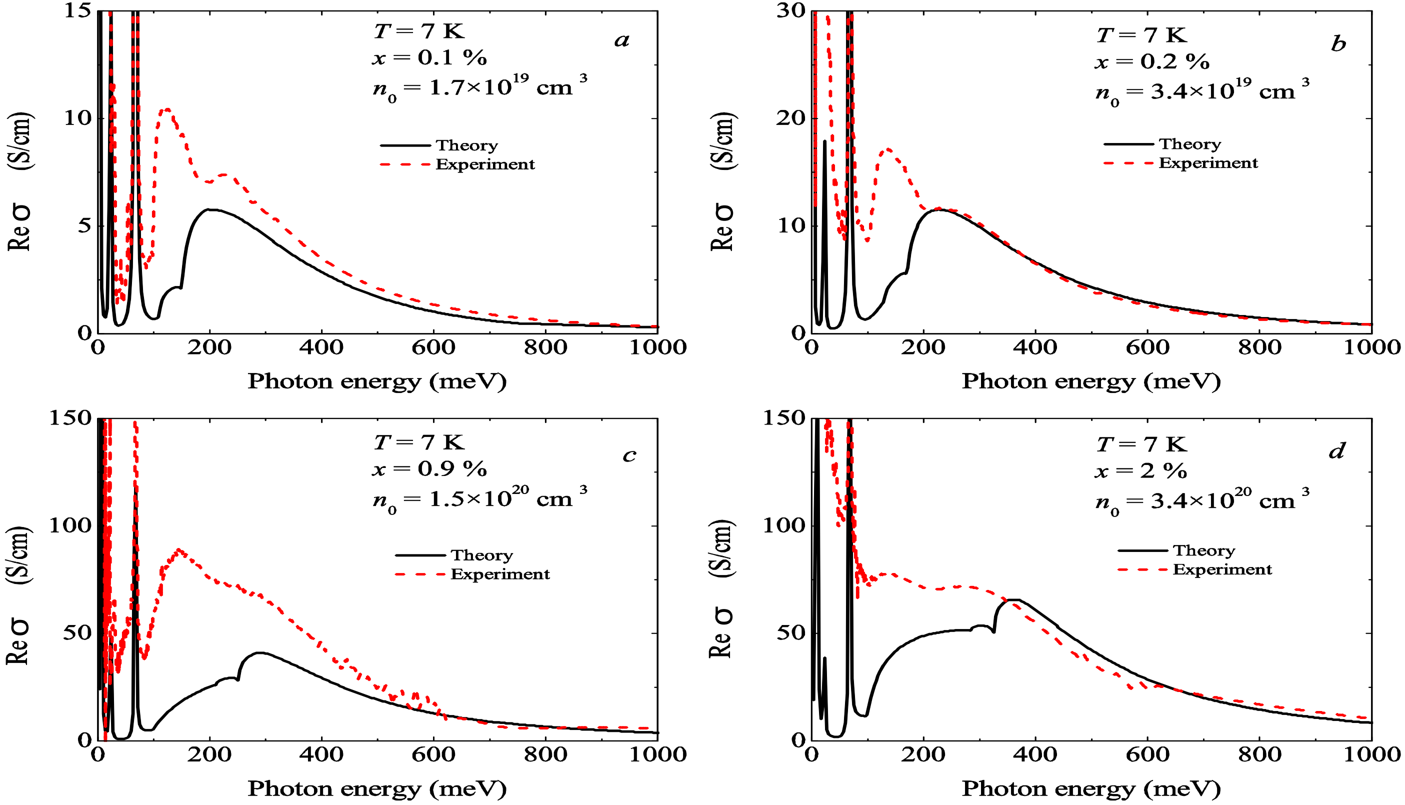
[1] *PRL* **100**, 226403 (2008)
[2] *NJ Ph* **12**, 023004 (2010)
[3] *PRB* **81**, 125119 (2010)
[4] *PRB* **84**, 205111 (2011)
[5] *PRB* **86**, 045113 (2012)
[6] *PRB* **89**, 184514 (2014)
[7] *Sc Rep* **6**, 37582 (2016)
[8] *J SC N Mag* **30**, 757 (2017)
[9] *PRB* **96**, 094518 (2017)
[10] *NatCom* **10**, 2774 (2019)
[11] *PRR* **1**, 013003 (2019)
[12] *In preparation* (2020)

Coupling to longitudinal optical phonons



Coupling to longitudinal optical phonons

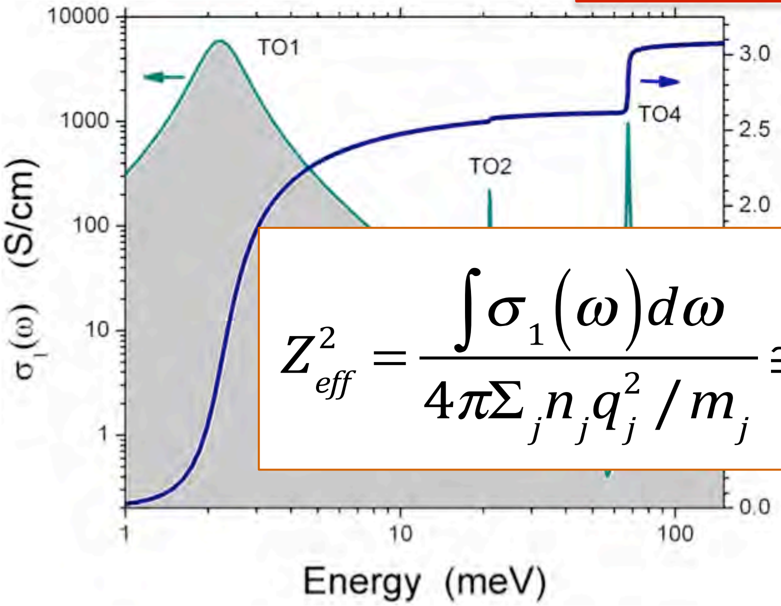
$\alpha_1 = 0.021$ $\alpha_2 = 0.46$ $\alpha_3 = 1.58$



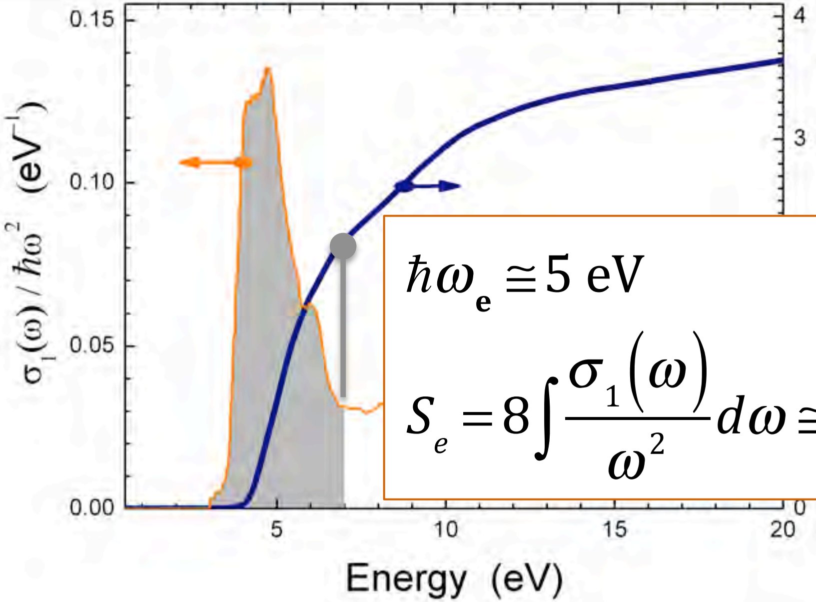
J.L.M. van Mechelen et al. , PRL100, 226403 (2008) & *J.T. Devreese et al., PRB 81 (2010) 125119*

Coupling to transverse optical phonons: "charged[1]" phonons

$$\hat{H} = \hbar\omega_n \hat{a}^\dagger \hat{a} - g\left(\hat{a}^\dagger + \hat{a}\right)\left(\hat{d}^\dagger \hat{p} + \hat{p}^\dagger \hat{d}\right) + \hbar\omega_e\left(\hat{d}^\dagger \hat{d} - \hat{p}^\dagger \hat{p}\right)/2$$



$$Z_{eff}^2 = \frac{\int \sigma_1(\omega)\, d\omega}{4\pi\Sigma_j n_j q_j^2 / m_j} \cong 3.1$$



$$\hbar\omega_{\mathbf{e}} \cong 5 \text{ eV}$$

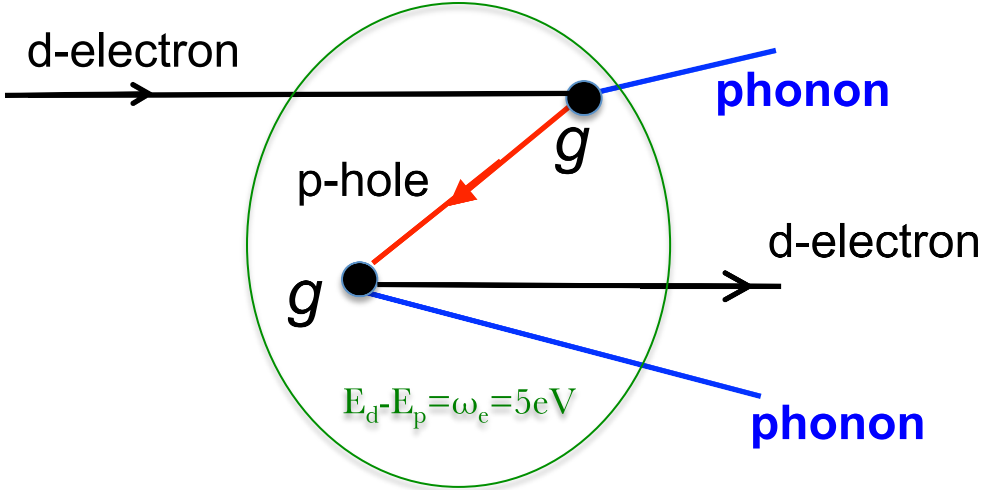
$$S_e = 8\int \frac{\sigma_1(\omega)}{\omega^2} d\omega \cong 2.2$$

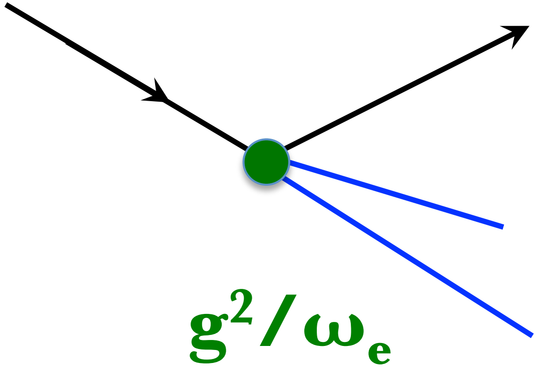
coupled oscillators $\Big\}$ $$g = \hbar\left(Z_{eff}^2 - 1\right)\sqrt{\frac{8\pi n_{pe} e^2 \omega_e}{m_n \omega_n}} \cong 0.57 \text{ eV}$$

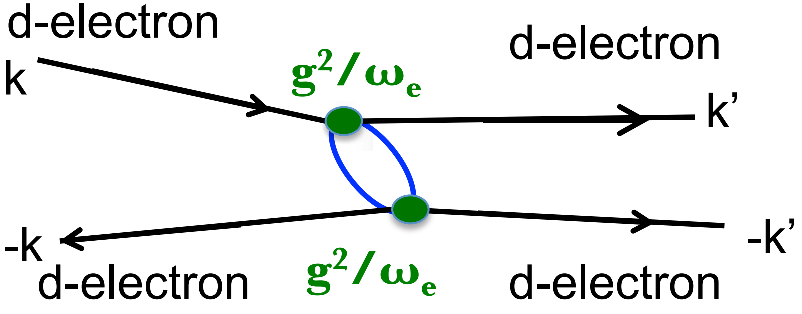
*[1] M.J.Rice, Lipari, Strässler, PRL **39**, 1359 (1977)*

*DvdM, F.Barantani, W.Rischau, PRR **1**, 013003 (2019)*

Coupling to transverse optical phonons







$$\lambda_{2ph} = \frac{g^4}{\tilde{\omega}_n \omega_e^2} D^*\left(\varepsilon_F\right)$$

Electron pairing mediated by TO bi-phonons

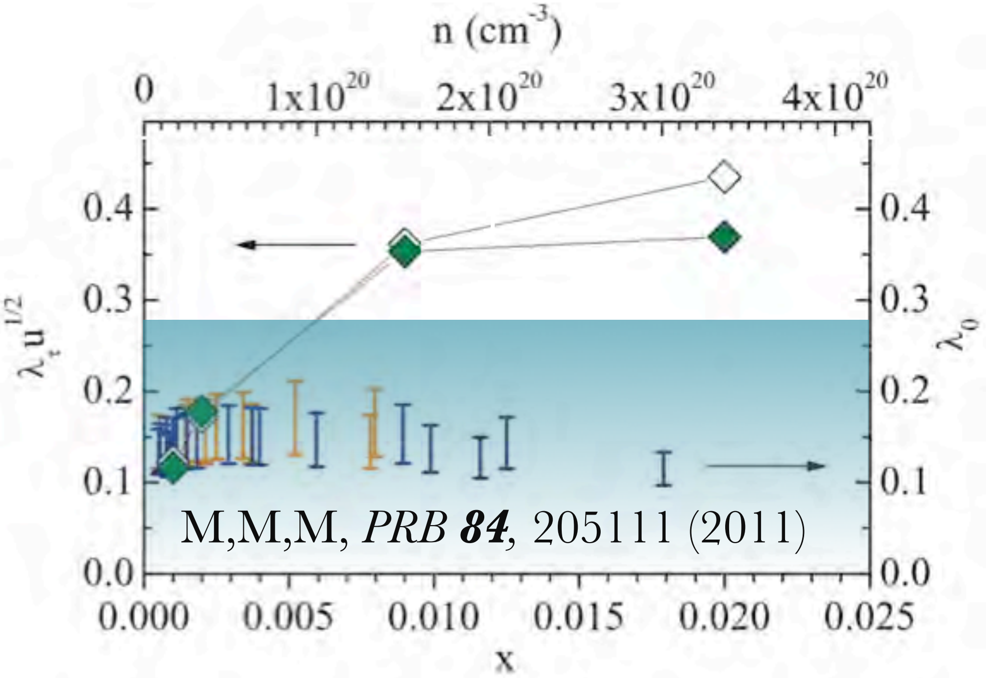
$$\lambda_{2ph} = \frac{g^4}{\tilde{\omega}_n \omega_e^2} D^*\left(\varepsilon_F\right)$$

$$\left.\begin{array}{l} g \approx 0.57\ eV \\ \omega_e \approx 5\ eV \\ \tilde{\omega}_n \approx 12\ meV \\ D^*\left(\varepsilon_F\right) \leq 0.8\ eV^{-1} \end{array}\right\} \lambda_{2ph} \leq\ 0.28$$

λ from experimental data

λ_0 : from T_c

λ_τ : from T^2 resistivity coefficient



M,M,M, *PRB* ***84***, 205111 (2011)

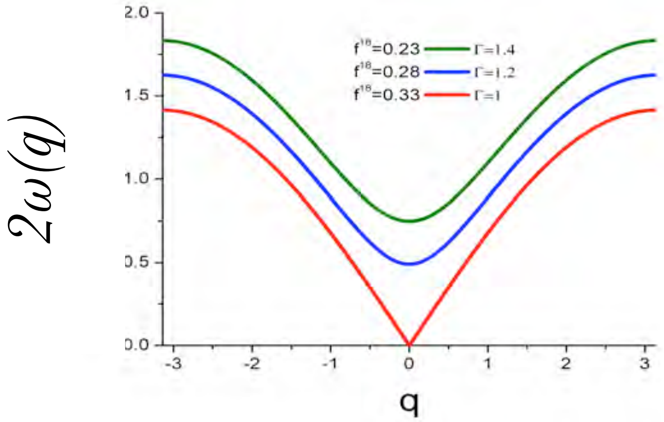
Pairing in doped STO mediated by soft ferro-electric phonons

2-phonon pairing: { k ; $-k$} → { $k-q-q'$; $-k+q+q'$ }

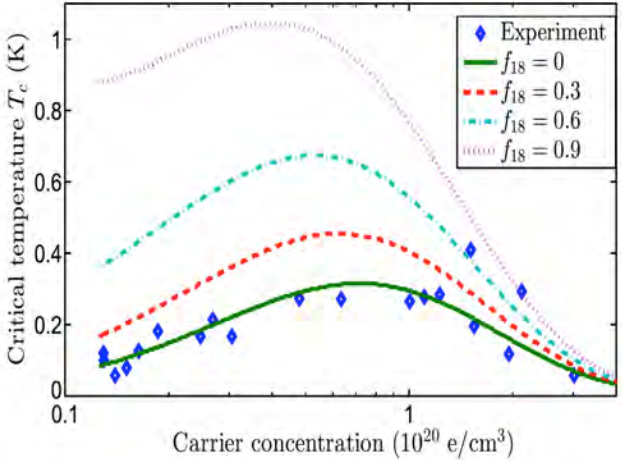
k and $k-q-q'$ are in a narrow shell around k_F
Low doping then implies: $|q+q'| << \pi$

=> $|\omega(q)-\omega(q')| << \omega(\pi)$

The phonons are the same ones as *in JM Edge et al, PRL 115, 247002 (2015)*.
Instead of $\omega(q)$: {$\omega(q)$; $\omega(-q)$} pairs.



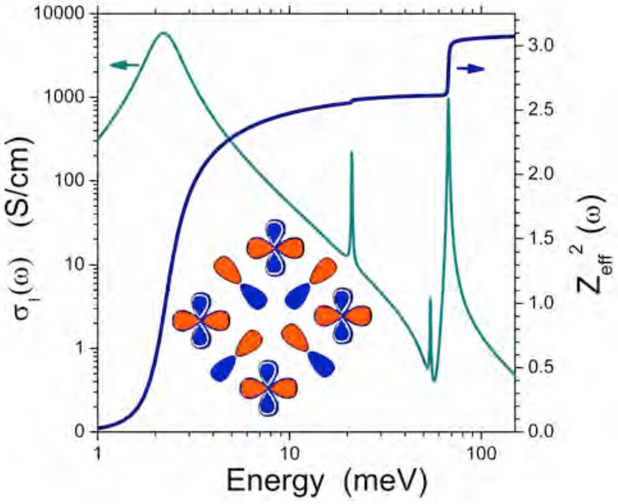
=>



Conclusions

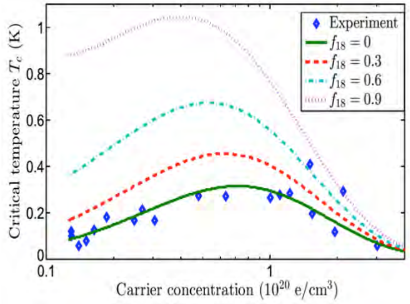
-Pairing is mediated by 2 transverse optical phonons with $q' = -q - k + k'$ and $\omega(q') \approx \omega(q)$

-The coupling constant can be calculated from the charged phonon effect in undoped $SrTiO_3$.



-Since the charged phonon effect is extremely strong in $SrTiO_3$, the e-2ph coupling constant is big enough to mediate the pairing. Back to Ngai, PRL 32 (1974).

-The charged phonon effect is even stronger in $KTaO_3$: $Z_{eff}^2 = 3.5$ (data in JAP 111,104101 (2012))



$T_c(^{18}O,n)$ phase diagram of Edge et al, PRL 115, 247002 (2015): All that is required is to replace $\omega(q)$ with $2\omega(q)$

This does not qualitatively change Edge et al's prediction

*DvdM, F Barantani, CW Rischau, Physical Review Research **1**, 013003 (2019)*