Theorie van Kwantumsystemen & Complexe Systemen
Universiteit Antwerpen

Workshop "Microscopics of Superconductivity in Perovskite Oxides: Challenges, Hurdles and Enigmas (MISPOCHE)" - 2020"
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Superconductivity and optical response of a many-polaron gas in $SrTiO_3$

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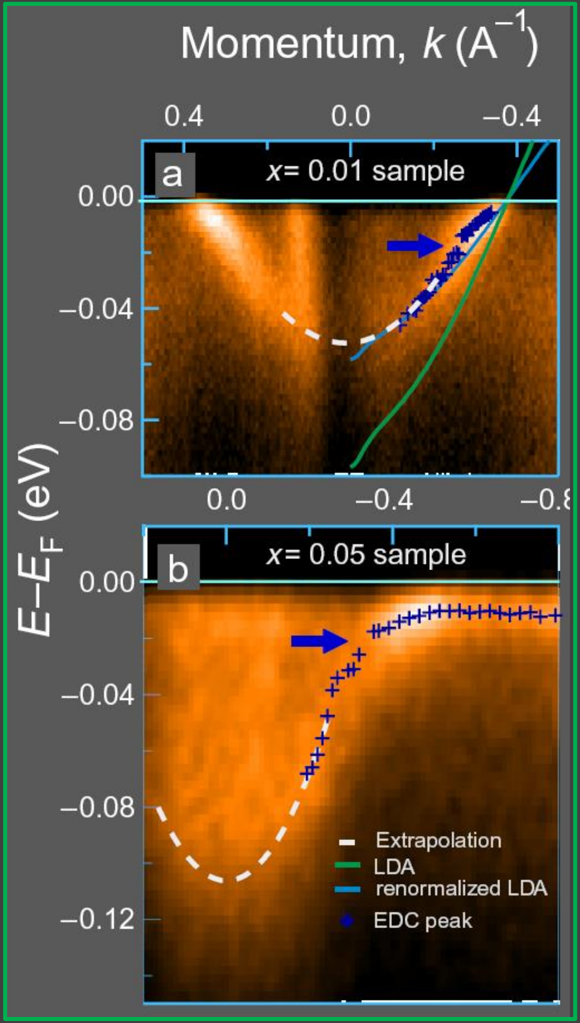
Renewed interest to $SrTiO_3$

- Band structure
- Electron-phonon interaction: large or small polarons?
- Superconductivity at low concentrations
- Optical response

Measurements of the effects of electron–phonon coupling using angle-resolved photoemission (ARPES) [1]

→ Direct evidence of the band energy spectrum

Optical conductivity: agreement with the large-polaron theory



[1] W. Meevasana *et al*., New J. Phys. **12**, 023004 (2010).
[2] J. L. M. van Mechelen *et al*., Phys. Rev. Lett. **100**, 226403 (2008)
[3] J. T. Devreese, SK, J. L. M. van Mechelen, and D. van der Marel, Phys. Rev. B **81**, 125119 (2010)

Dielectric function method

Account of a dynamic electron-phonon response

Dielectric function method: KMK [1]
extended for a multiband crystal with *non-parabolic* bands

$$\Delta_\lambda(\mathbf{p}) = -\frac{1}{(2\pi)^3}\int d\mathbf{k}\,\Delta_\lambda(\mathbf{k})\,\frac{\tanh\frac{\beta|\varepsilon_{\mathbf{k},\lambda}|}{2}}{2|\varepsilon_{\mathbf{k},\lambda}|} \times \frac{2}{\pi}\int_0^\infty d\Omega \frac{|\varepsilon_{\mathbf{k},\lambda}|+|\varepsilon_{\mathbf{p},\lambda}|}{\Omega^2+(|\varepsilon_{\mathbf{k},\lambda}|+|\varepsilon_{\mathbf{p},\lambda}|)^2} V^R(\mathbf{p}-\mathbf{k}, i\Omega)$$

DFT method for electron and phonon states: C. Franchini *et al.*, Phys. Rev. B **91**, 085204 (2015)

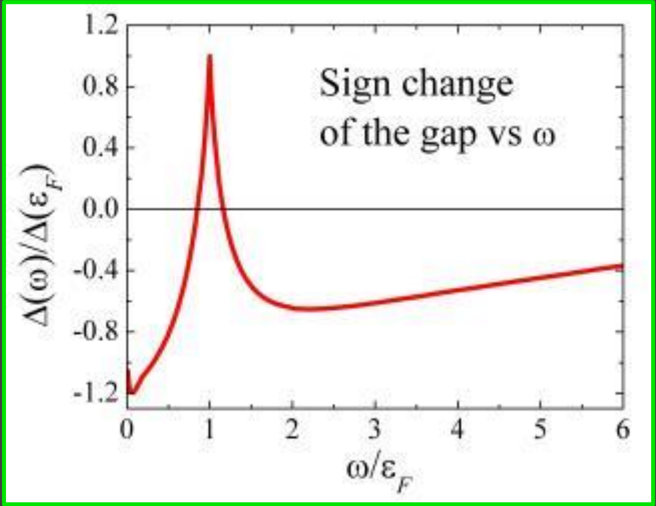
$$\varepsilon^R(q,i\Omega) = \varepsilon_\infty \prod_{j=1}^{n}\left(\frac{\Omega^2+\omega_{L,j}^2(q)}{\Omega^2+\omega_{T,j}^2(q)}\right) - \frac{4\pi e^2}{q^2}P^{(1)}(q,i\Omega)$$

The lowest-energy TO → Ferroelectric mode

The effective potential

$$V^R(\mathbf{q}, i\Omega) = \frac{4\pi e^2}{q^2\varepsilon^R(\mathbf{q}, i\Omega)}$$

is expressed through the total dielectric function constituted by both many-electron and phonon responses.



[1] D. A. Kirzhnits, E. G. Maksimov and D. I. Khomskii, J. Low Temp. Phys. **10**, 79 (1973).
[2] SK, J. Tempere, J. T. Devreese, and D. van der Marel, J. Sup. Nov. Magn. **30**, 757 (2017)
[3] B. Rosenstein *et al.*, Phys. Rev. B **94**, 024505 (2016)
[4] P Chandra *et al.* Rep. Prog. Phys. **80**, 112502 (2017)
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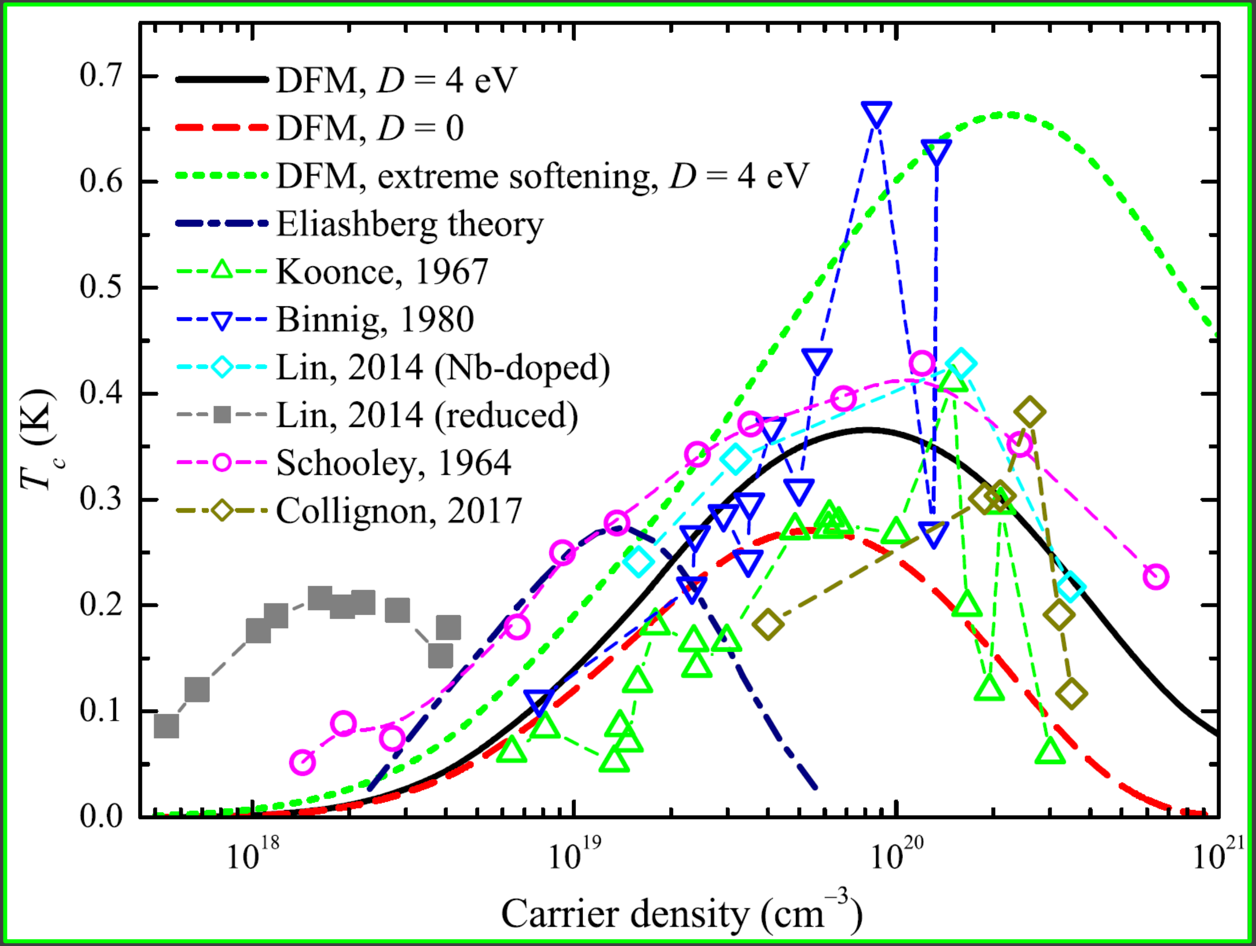
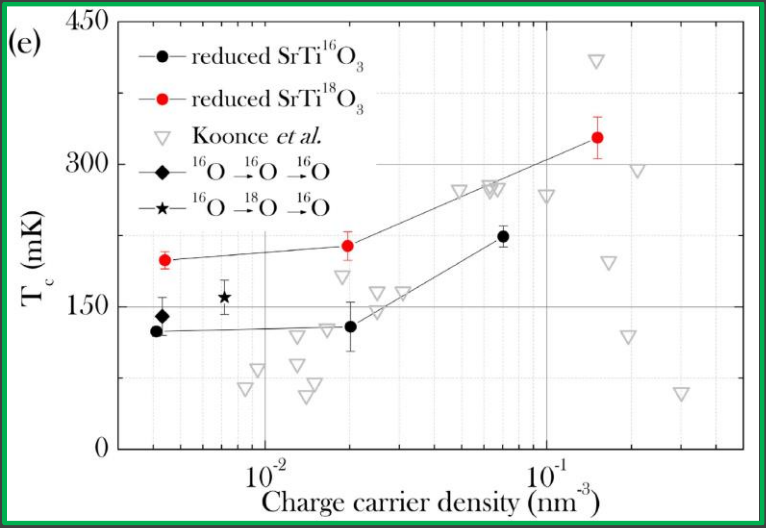
Dielectric function method (DFM) for superconductivity: application to bulk $SrTiO_3$



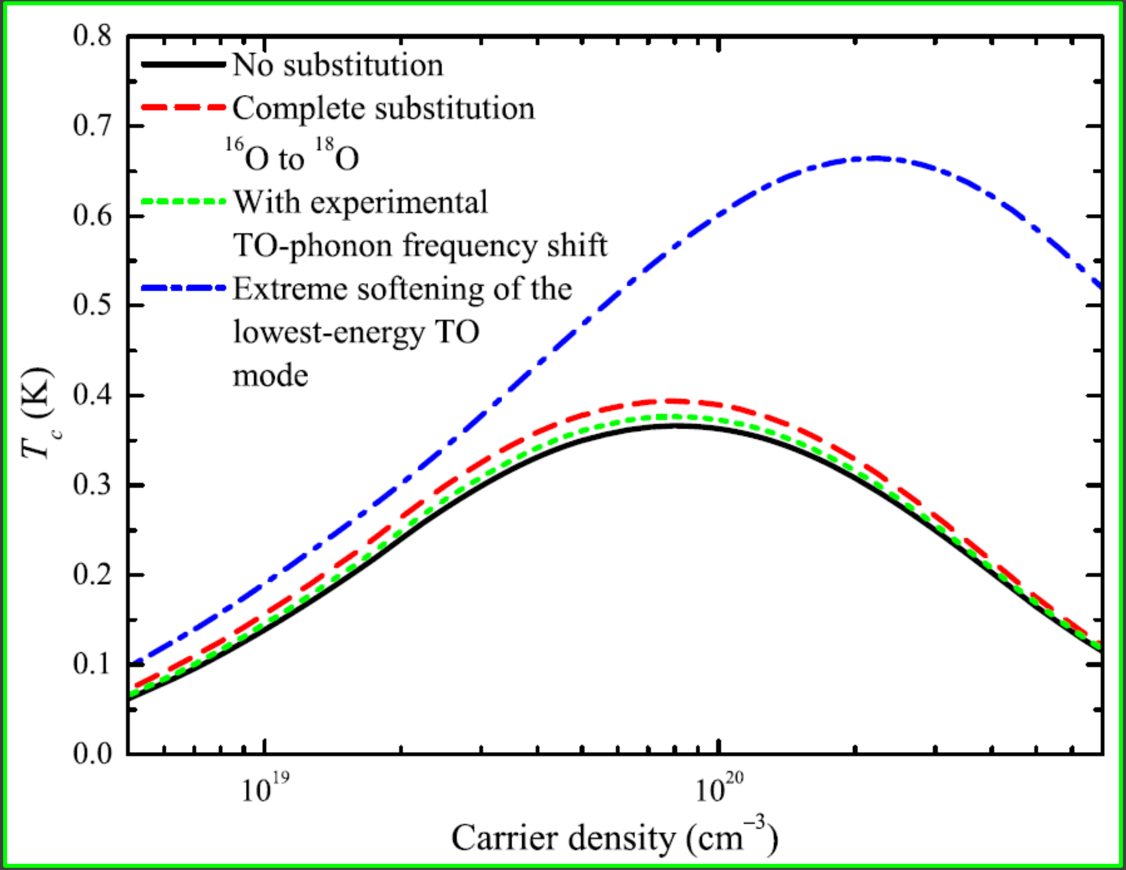
Using experimental parameters and the non-parabolic band structure of strontium titanate, the calculated dome-shaped density dependence of T_c is in agreement with experiments

SK, J. Tempere, J. T. Devreese, J. He, C. Franchini and G. Kresse, J. Sup. Nov. Magn. **32**, 2739 (2019)

Isotope effect in $SrTiO_3$



The observed isotope effect has a sign opposite to conventional superconductors



The dielectric function method predicts the correct sign of the isotope effect in $SrTiO_3$ due to softening of TO phonon modes.

SK, J. Tempere, J. T. Devreese, J. He, C. Franchini and G. Kresse, J. Sup. Nov. Magn. **32**, 2739 (2019)
Experiment: D. van der Marel et al., Sci. Rep. **6**, 37582 (2016)

Many-polaron optical response

The optical conductivity in the memory-function form using :

$$\sigma_{xx}(\Omega) = \frac{i}{V}\frac{\mathcal{Z}}{\Omega + i\delta - \chi(\Omega)/(\Omega + i\delta)}$$

with the normalization constant accounting for band nonparabolicity

$$\mathcal{Z} = \frac{e^2}{\hbar^2}\sum_{\lambda}\sum_{\mathbf{k}}\sum_{\sigma}\frac{\partial^2 \varepsilon_\lambda(\mathbf{k})}{\partial k_x^2} f_{\mathbf{k},\sigma,\lambda}$$

The memory function is expressed through the force-force correlation function

$$\chi(\Omega) = -\frac{i}{\mathcal{Z}}\frac{e^2}{\hbar}\int_0^\infty dt\, e^{-\delta t}\left(e^{i\Omega t} - 1\right)\langle[\mathcal{F}_x(t), \mathcal{F}_x(0)]\rangle_0$$

The correlation function is calculated within RPA taking into account the dynamic screening

J. T. Devreese, SK, J. L. M. van Mechelen, and D. van der Marel, Phys. Rev. B **81**, 125119 (2010)
SK, J. Tempere, J. T. Devreese, C. Franchini and G. Kresse, Appl. Sci. **10**, 2059 (2020)

$SrTiO_3$: Many-polaron optical conductivity accounting for dynamic screening

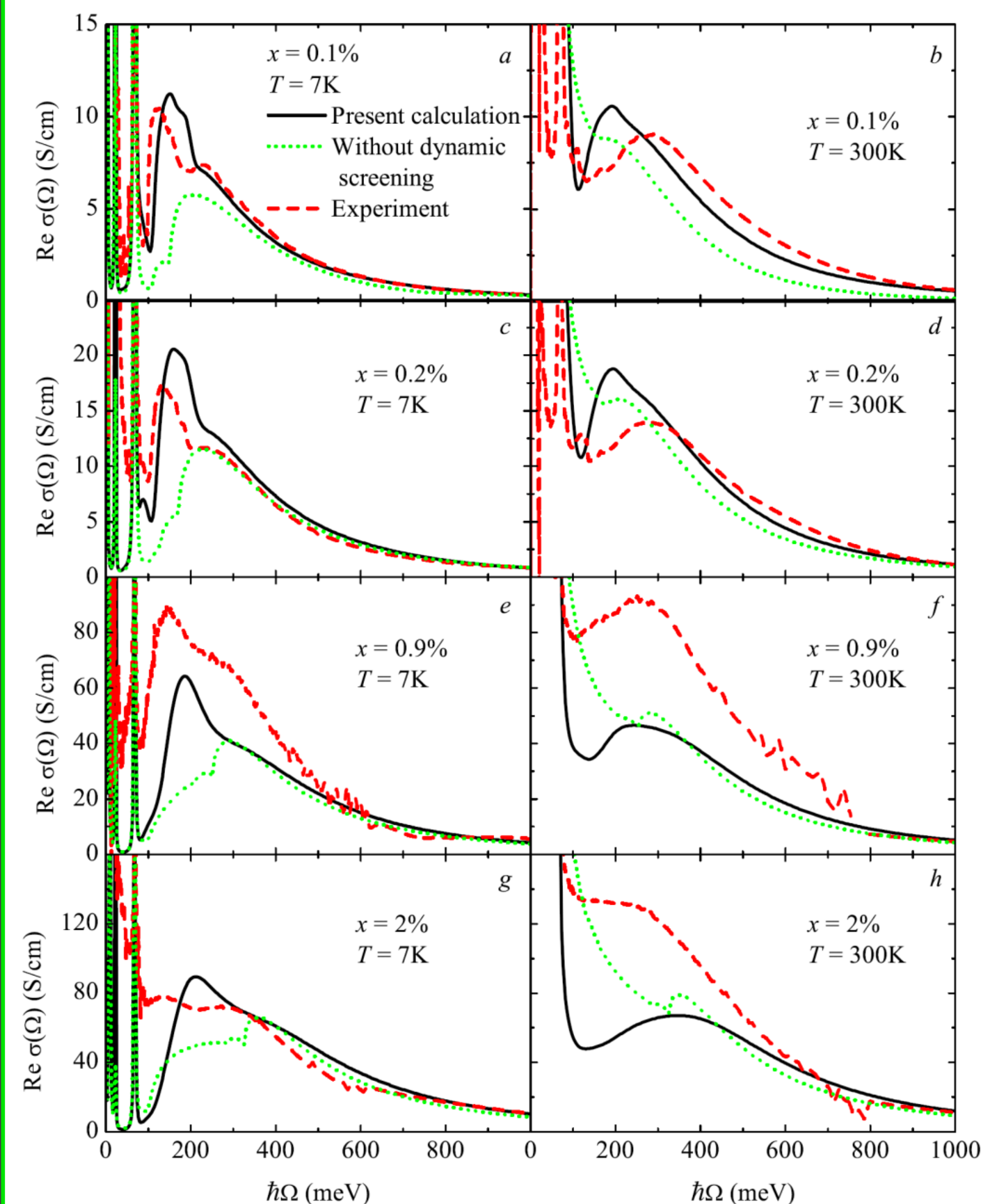
Large-polaron optical conductivity spectra [1, 2] in comparison with the experimental data [3]

Many-body effects are taken into account

The density-of-states approximation [1]:

$\varepsilon_\lambda(\mathbf{k}) \rightarrow \varepsilon_\lambda(k)$ with the same density of states as for $\varepsilon_\lambda(\mathbf{k})$.

The low-energy feature appears due to the dynamic screening of the Coulomb interaction by LO phonons



[1] J. Tempere and J. T. Devreese, Phys. Rev. B **64**, 104504 (2001)
[2] J. T. Devreese, SK, J. L. M. van Mechelen, and D. van der Marel, Phys. Rev. B **81**, 125119 (2010)
[3] SK, J. Tempere, J. T. Devreese, C. Franchini and G. Kresse, Appl. Sci. **10**, 2059 (2020)
[4] J. L. van Mechelen, D. van der Marel, C. Grimaldi, A. B. Kuzmenko, N. P. Armitage, N. Reyren, H. Hagemann, and I. I. Mazin, Phys. Rev. Lett. **100**, 226403 (2008)

Conclusions

- The dielectric function method is capable to interpret superconductivity in strontium titanate.
- Many-polaron optical conductivity in $SrTiO_3$ has been revisited.
- The shape of the many-polaron optical conductivity spectrum is explained within the density-of-states approach, including the 130-meV feature without involving additional mechaniisms