# Resonant States, Quantum Confinement : Engineering Electronic Transport

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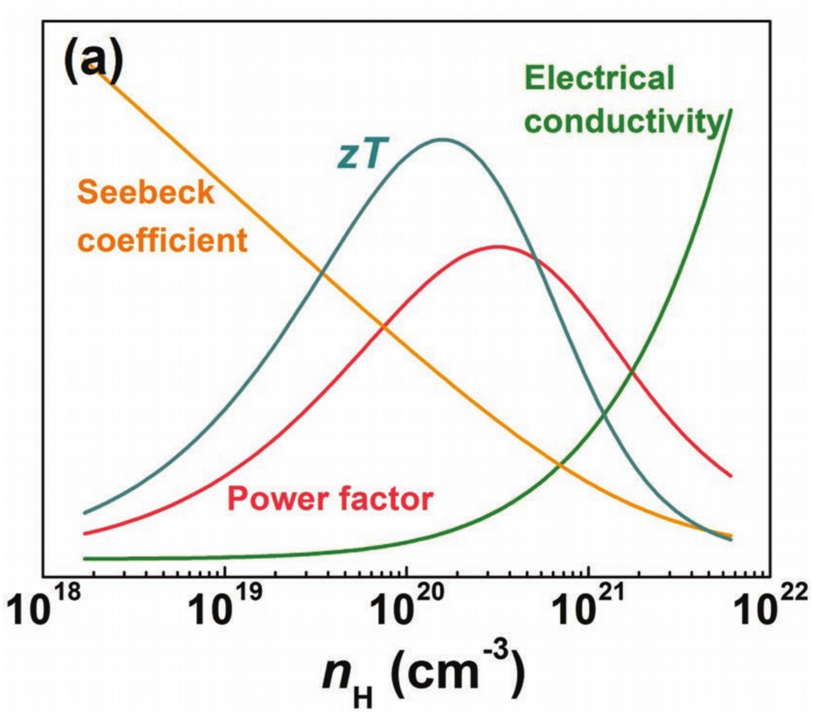
# Introduction

Thermoelectric figure of merit : $ZT = \frac{\sigma S^2 T}{\kappa}$

**Power Factor** governed by electronic transport




From T. Zhu et al.,
Adv. Mater. 2017, 29, 1605884

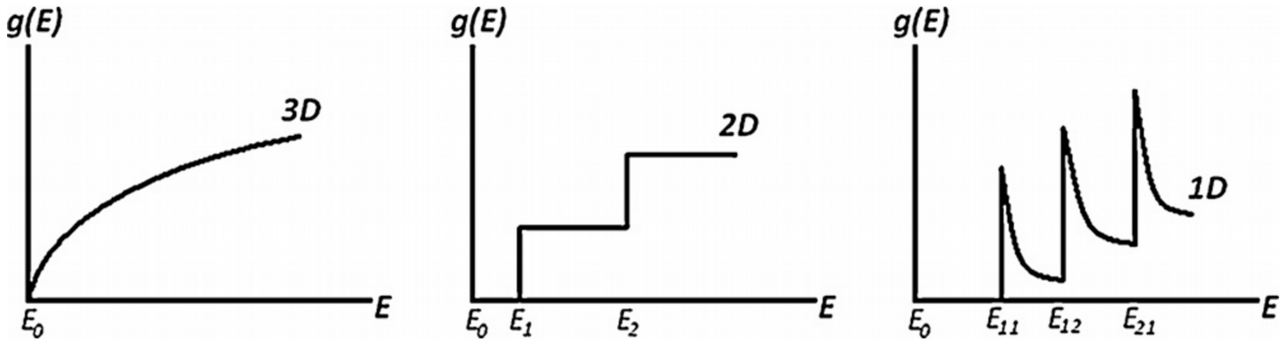
Typical state-of-the-art Power Factors :

- BiSbTe alloy
  20-40 $\mu W.cm^{-1}.K^{-2}$
- La/Nb doped $SrTiO_3$
  30-40 $\mu W.cm^{-1}.K^{-2}$

# Overview : quantum confinement

- Idea : reducing the dimensionality to enhance the DOS

  Expectation : larger, steeper DOS ⟶ boost of σ and S

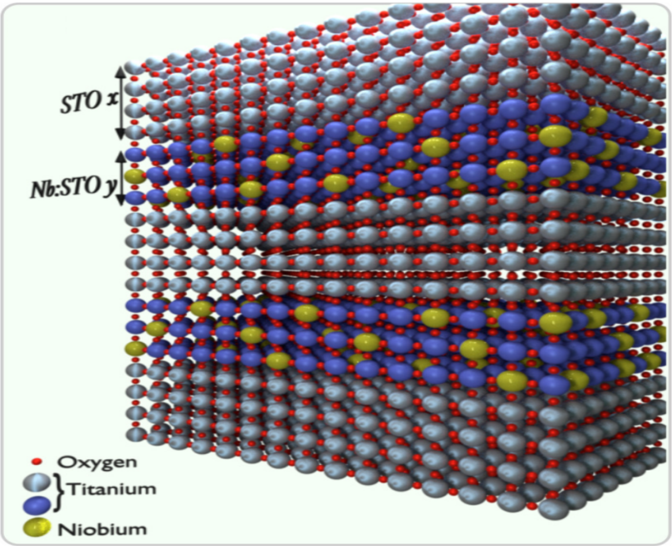



From P. Pichanusakorn and P. Bandaru, Mat. Science and Engineering R 67 (2010) 19

- In practice : **Superlayers**

  Ex : $SrTiO_3$/Nb:$SrTiO_3$

  by Ohta et al.

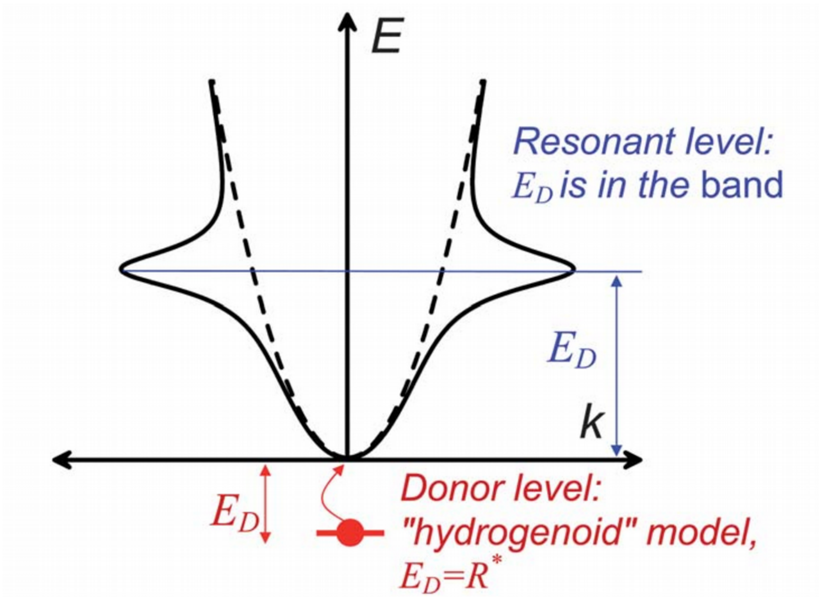



From G. Bouzerar et al., submitted

# Overview : resonant states

- Idea : creating impurity states inside the conduction band

  Expectation : **Sharp peak** in the DOS ⟶ boost of σ and S




From J. P. Heremans, B. Wiendlocha and A. M. Chamoire, Energy Environ. Sci., 2012, 5, 5510

- Many attempts (Tl:PbTe, Sn:BiTe, In:SnTe...)

- **BUT** : narrow peak in the DOS ⟶ **localized states**

# Tight-binding model for resonant states

- Simple cubic lattice
- 1 conduction band + 1 impurity band
- Constant relaxation time approximation

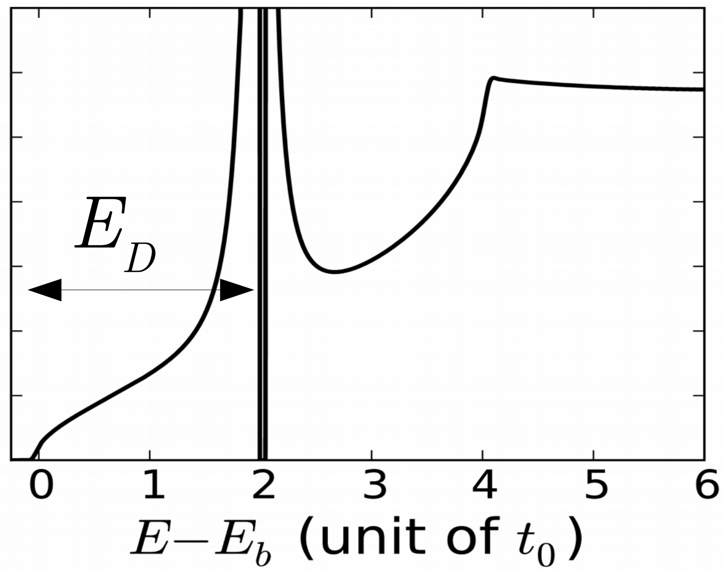
$$H = -t_0 \sum_{<i,j>} \left( c_i^\dagger c_j + c_j^\dagger c_i \right) + E_D \sum_i l_i^\dagger l_i + V \sum_i \left( l_i^\dagger c_i + c_i^\dagger l_i \right)$$

Extended conduction state

Heavy resonant state

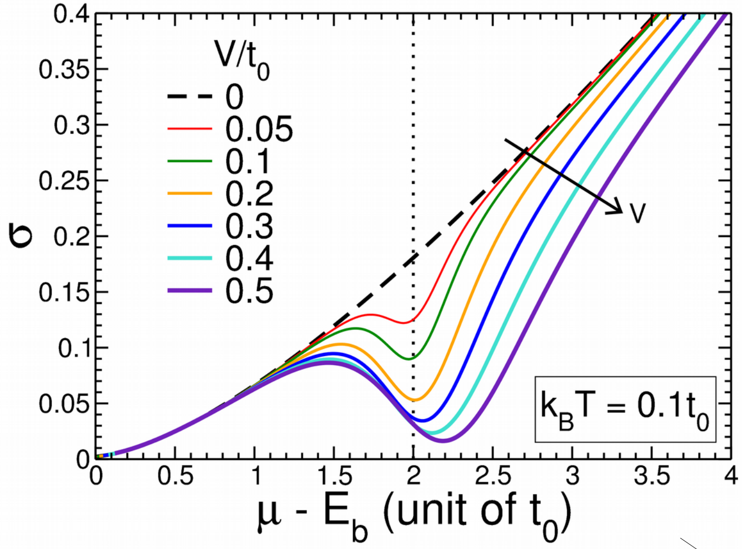
Hybridization

**Sharp peak in the DOS :**

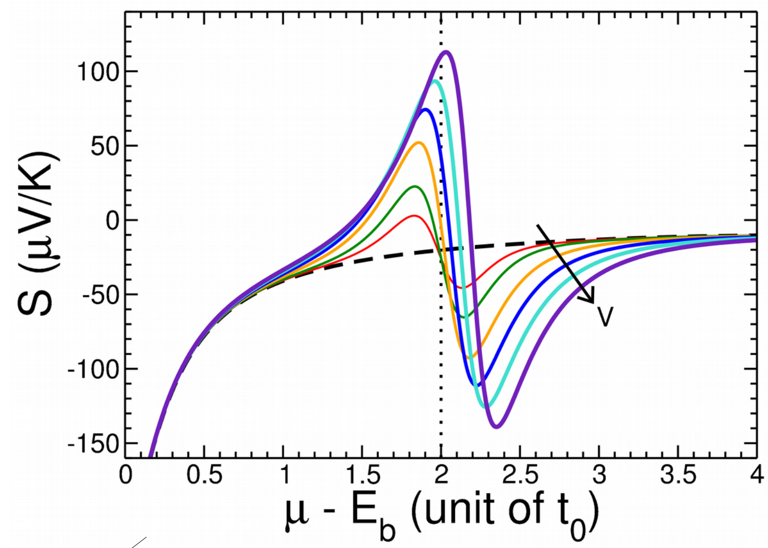


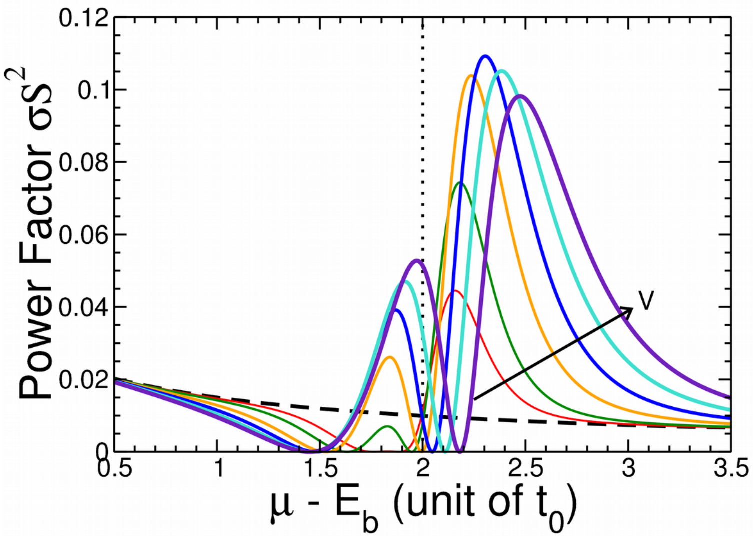

From S. Thébaud, C. Adessi, S. Pailhès and G. Bouzerar, Phys. Rev. B 96, 075201 (2017)

# Tight-binding model for resonant states




σ is
suppressed
but S
can be boosted

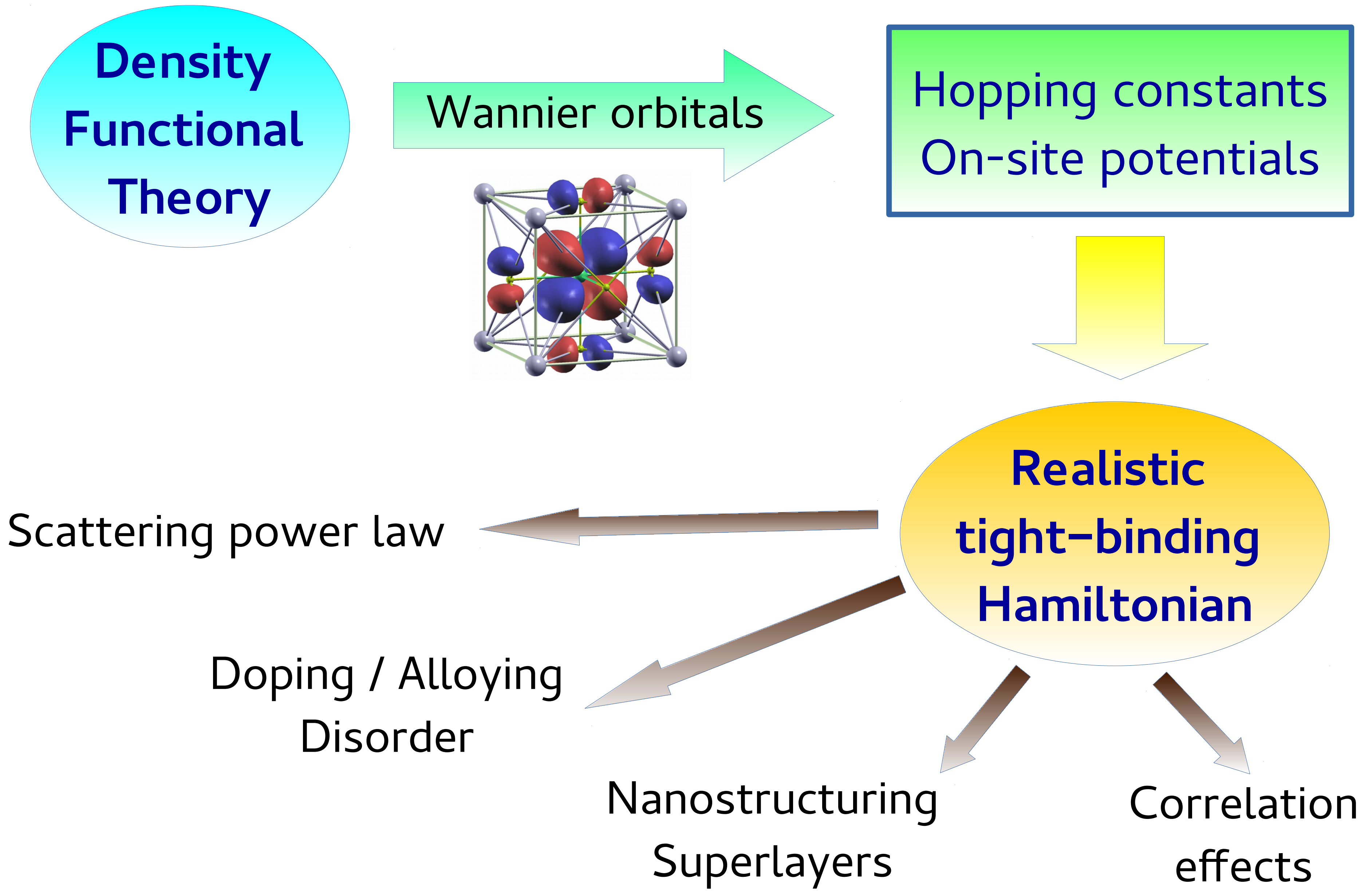



**Power Factor can be boosted !**

From S. Thébaud, C. Adessi, S. Pailhès and G. Bouzerar, Phys. Rev. B 96, 075201 (2017)

# Realistic models : hybrid approach

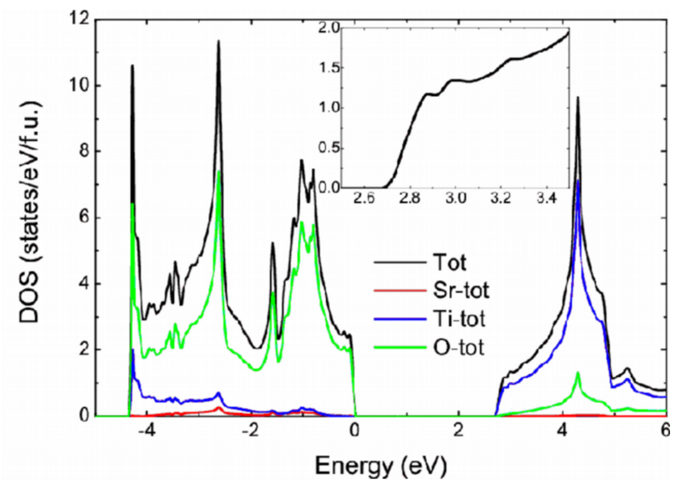


# Realistic tight-binding model for $SrTiO_3$

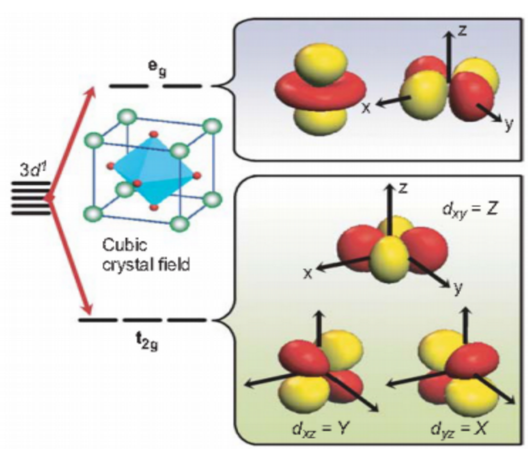
<u>DFT</u> :

Conduction band from

Ti $3d_{xy}$, $3d_{xz}$, $3d_{yz}$ orbitals




From J. Sun and D. J. Singh., APL Mater. 4, 104803 (2016)



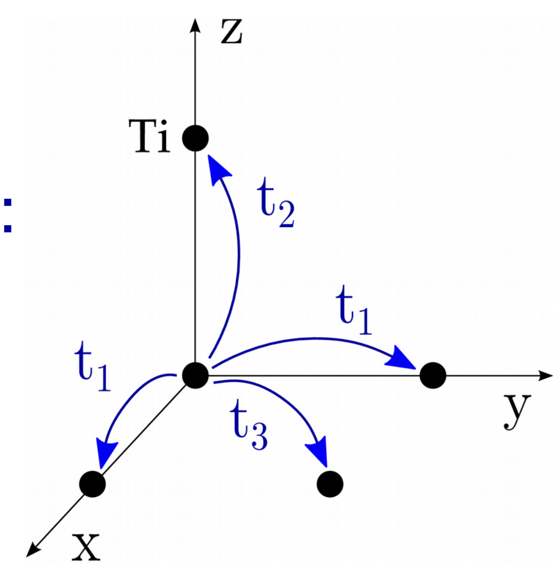

From T. Yildirim et al., NCNR 2003 Annual Report

<u>Wannier</u> :

3 hopping terms Between Ti atoms

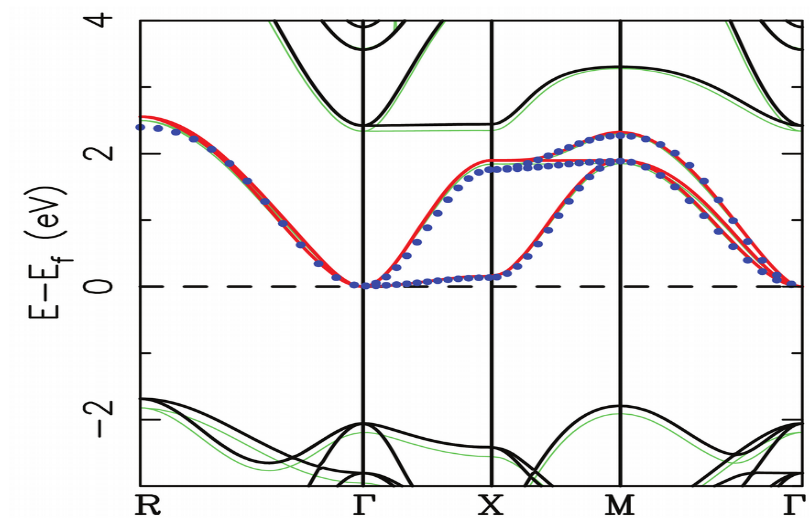
- $t_1$ = 0.28 eV
- $t_2$ = 0.031 eV
- $t_3$ = 0.076 eV

$3d_{xy}$ :



# Realistic tight-binding model for $SrTiO_3$

**Band structure :**




From G. Bouzerar et al., EPL 118 (2017) 67004

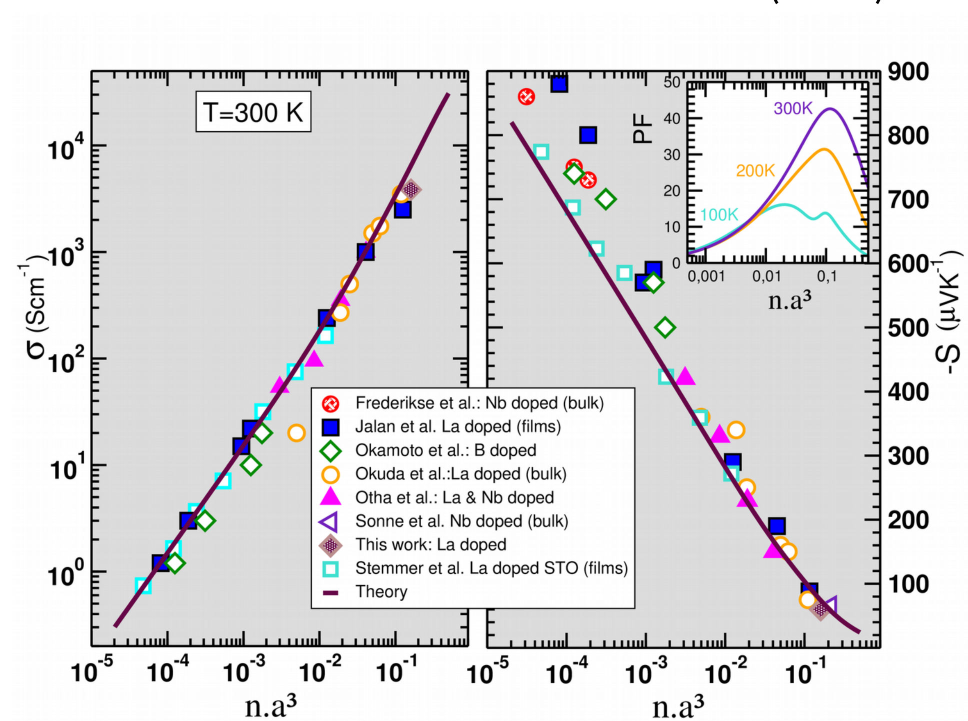
**Transport properties :**

Disorder scattering

$$\frac{\hbar}{\tau_{dis}} = \frac{\pi W^2}{6}\rho(E)$$

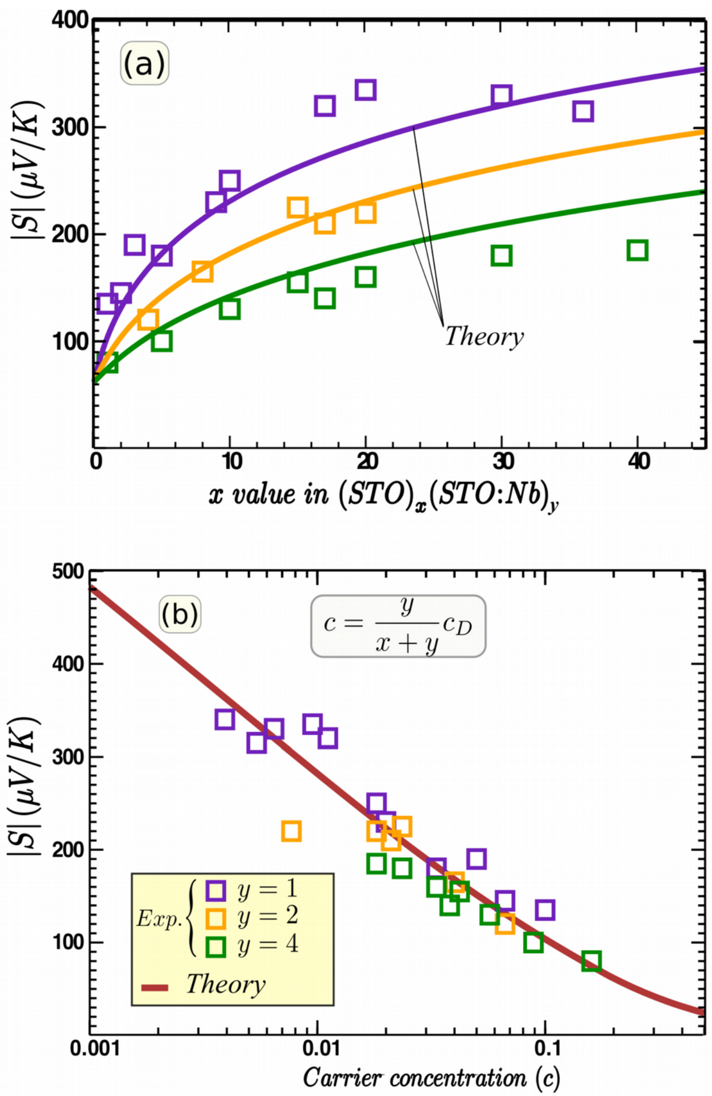
Electron-electron scattering

$$\frac{\hbar}{\tau_{e-e}} = \frac{C(k_B T)^2}{E - E_b}$$

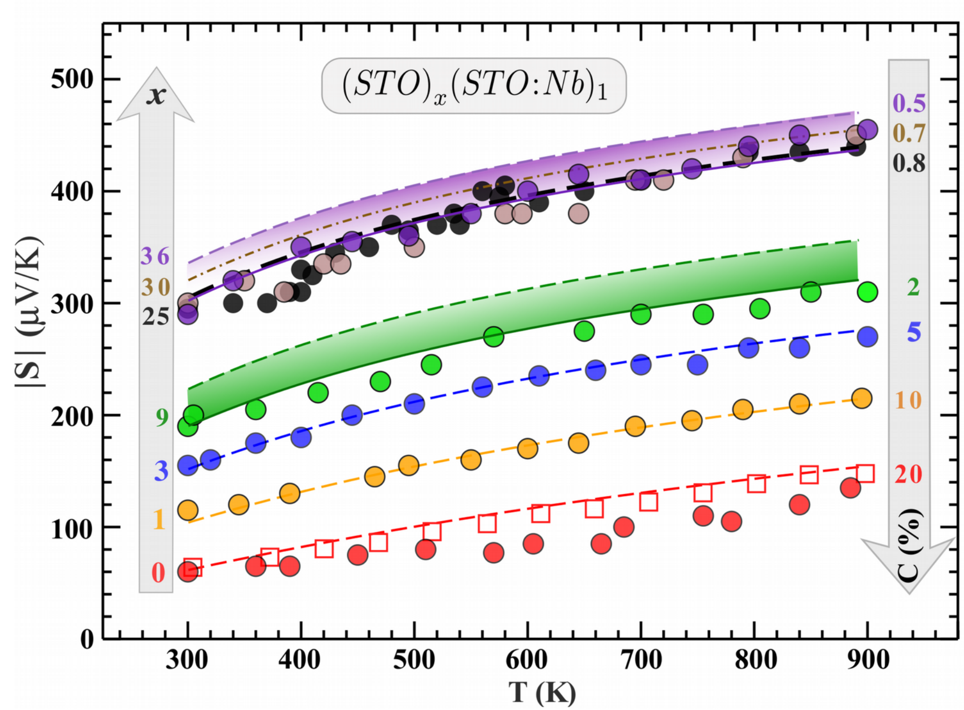


# Confinement in $(STO)_x(Nb{:}STO)_y$ superlayers ?

Nb doped layers : $c_D$ = 20 %




From G. Bouzerar et al., submitted




Theory for <u>bulk</u> STO predicts results for supperlattice !

**No quantum confinement…**

# Conclusions

- **Powerful hybrid approach** :
  DFT → Wannier → realistic tight-binding model
  Perspectives : TiO2, NbFeSb...

- **Resonant states :**
  Boost of power factor despite drop in conductivity

- **Confinement in superlattices :**
  Quantum confinement needs careful checking