Exchange enhancement of electron-phonon interactions in rhombohedral graphene

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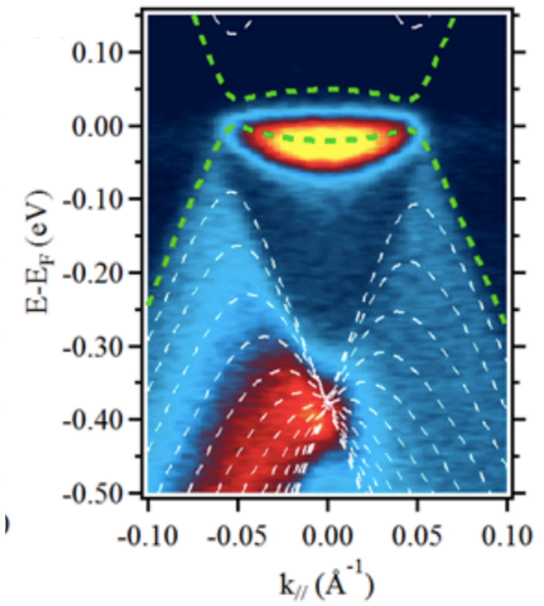
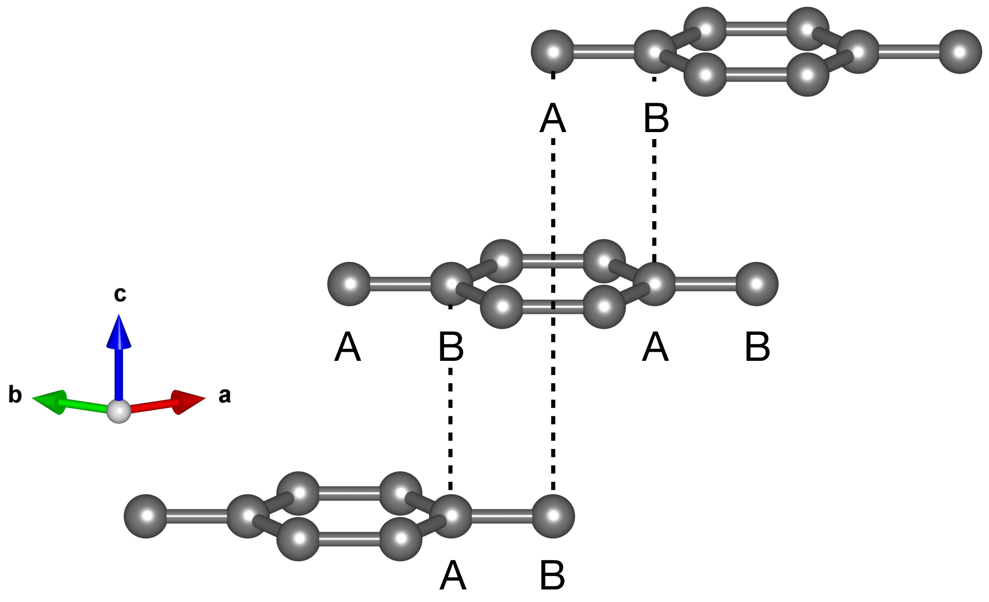
Strongly correlated phases in rhombohedral-stacked graphene

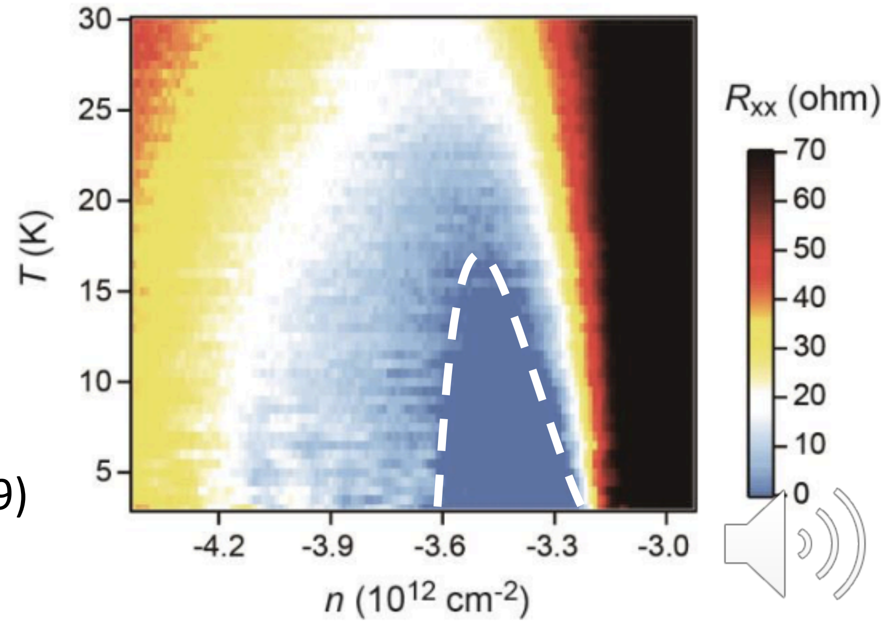


From first-principles calculations it is possible to identify an antiferromagnetic ground state with a band gap of about 40 meV due to electron-electron interaction, compatible with experiments.

H. Henck et al., Phys. Rev. B **97**, 245421 (2018)

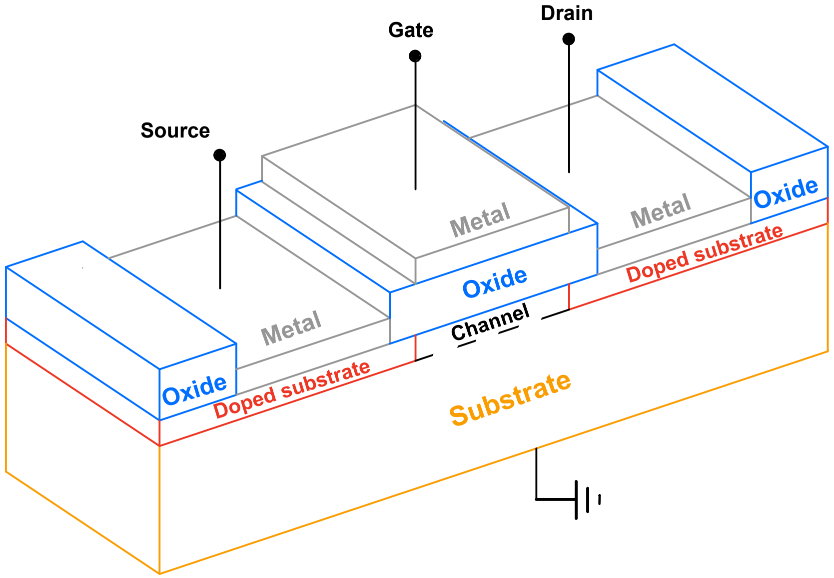


When stacking rhombohedral graphene on top of hexagonal boron nitride and upon electrostatic doping, a SC dome was observed with a Berezinskii–Kosterlitz–Thouless transition up to T_{BKT} = 14 K.

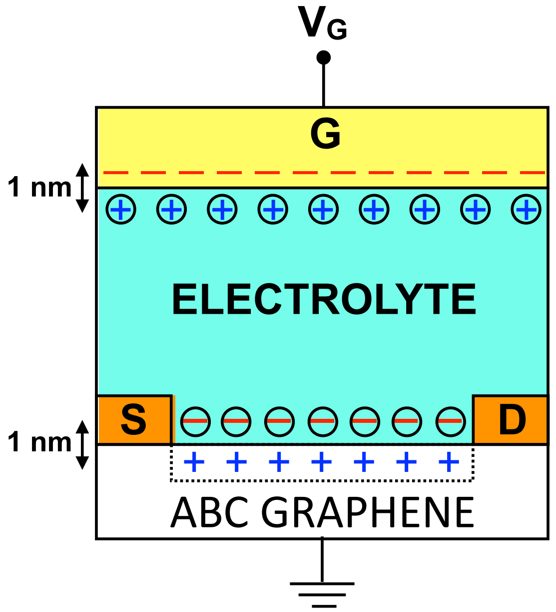


S. Moriyama et al., arXiv:1901.09356 **[cond-mat.supr-con]** (2019)

Field-effect doping



- Effective doping of the first layers of the sample (either electrons or holes);
- Avoids the introduction of impurities and leads to a quasi-2D system;
- The amount of charge induced by ionic liquid ($10^{14} \div 10^{15}$ cm^{-2}) is one or two orders of magnitude higher than solid state dielectric (10^{13} cm^{-2});



Key features of the DFT-implemented FET model

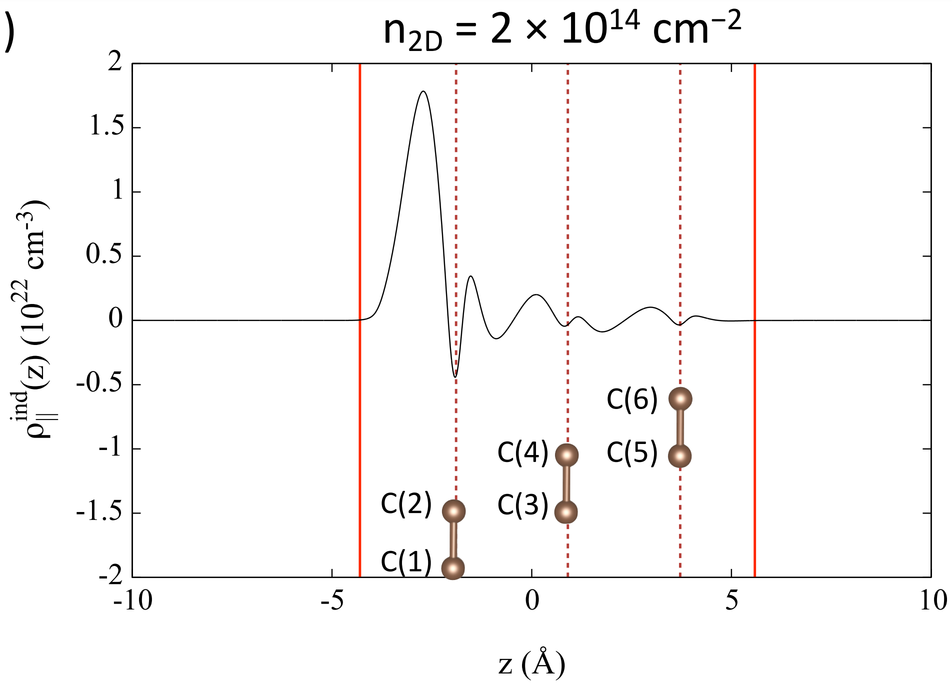
[Th. Sohier, M. Calandra and F. Mauri, Phys. Rev. B **96**, 075448 (2017)]

- Ionic layer → sheet of uniformly distributed charges;
- Potential barrier which prevents charge spilling;
- Coulomb interaction truncated along the direction perpendicular to the sample surface.

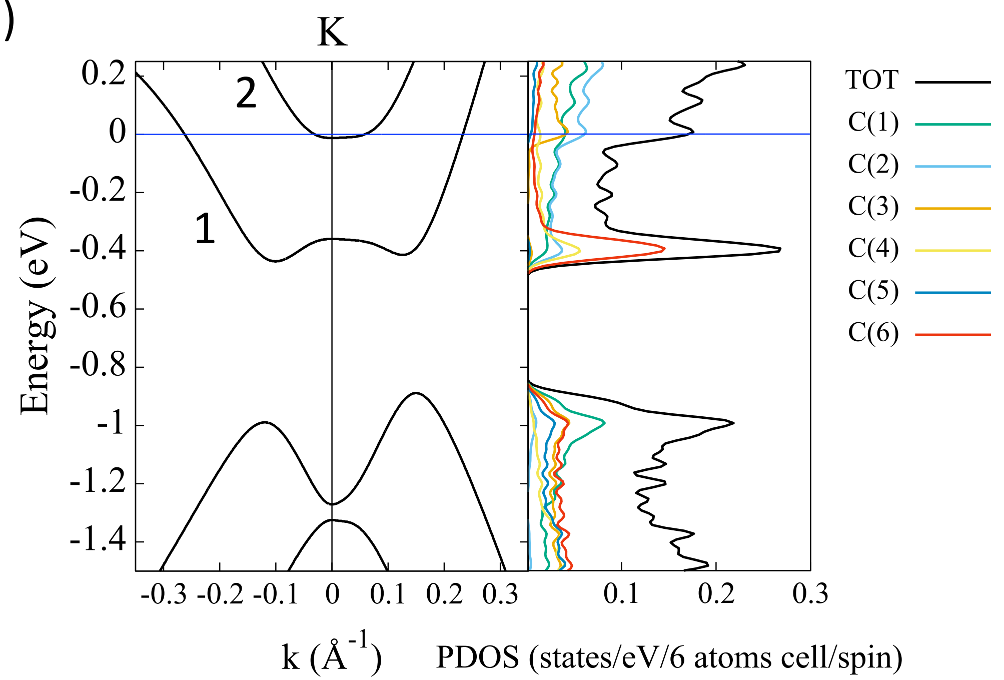
G →Gate
S →Source
D →Drain

Electronic structure

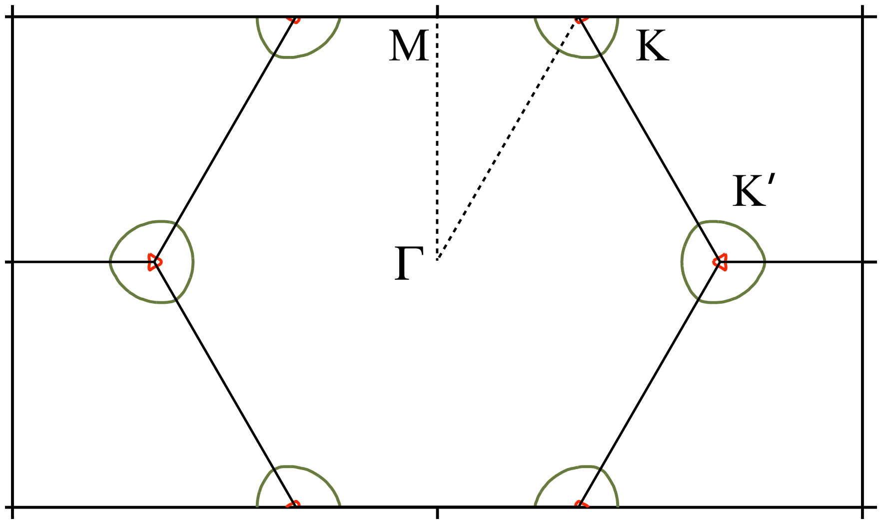
(a)



(b)



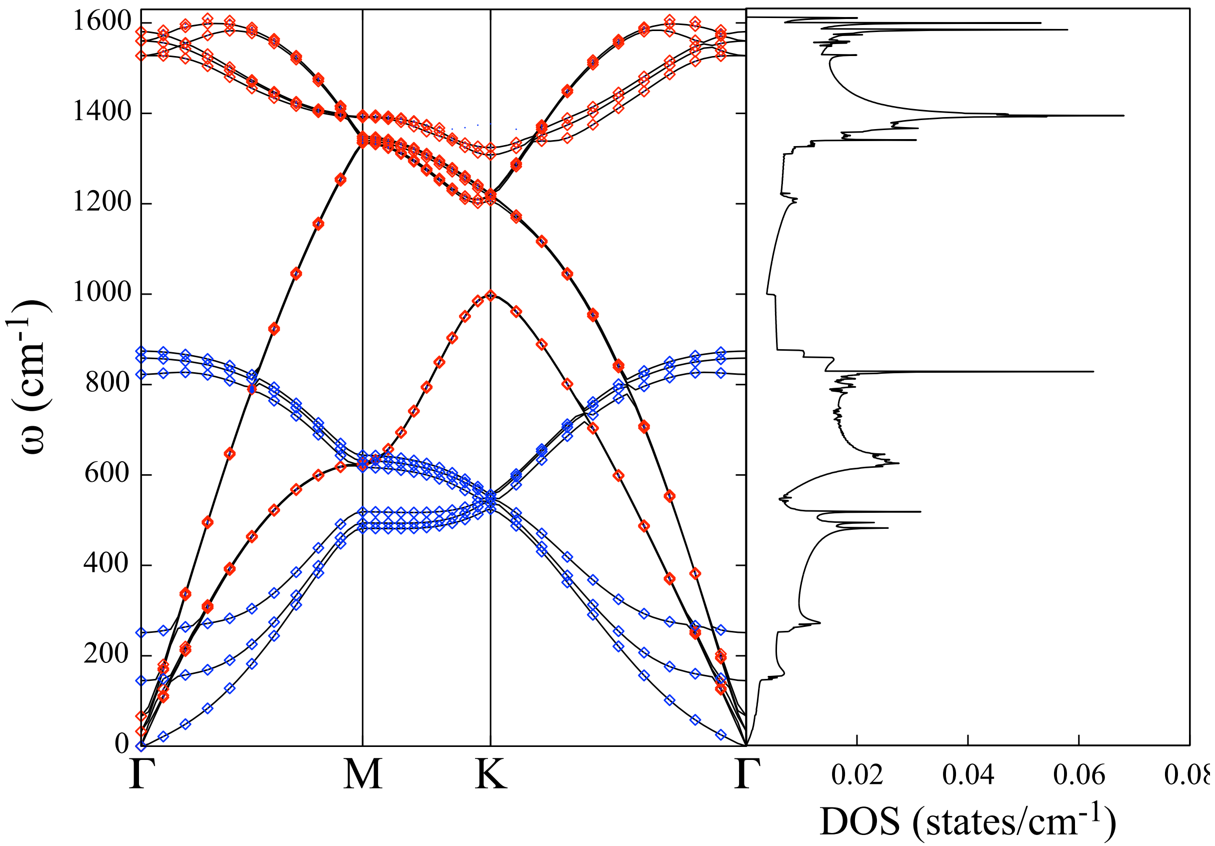
(c)

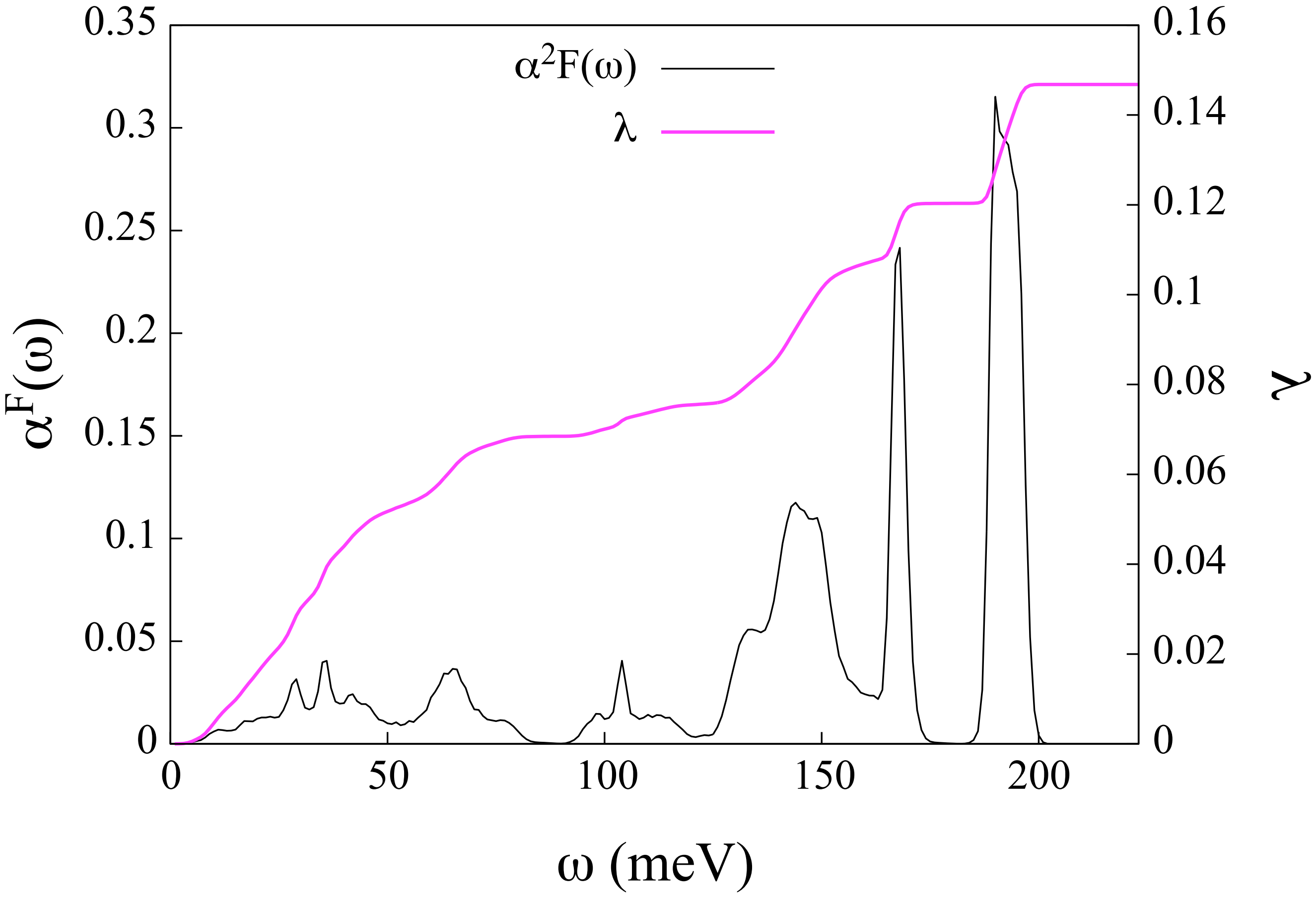


- The induced charge density is concentrated on the first layer;
- The first two carbon atoms (C(1) and C(2)) contribute to the van Hove singularity at the Fermi level;
- The Fermi surface consists of two concentric electron pockets centered around **K** and **K'**.

Vibrational properties and superconductivity

Wannier interpolation of e-ph matrix elements:
M. Calandra, G. Profeta, and F. Mauri, Phys. Rev. B **82**, 165111 (2010)

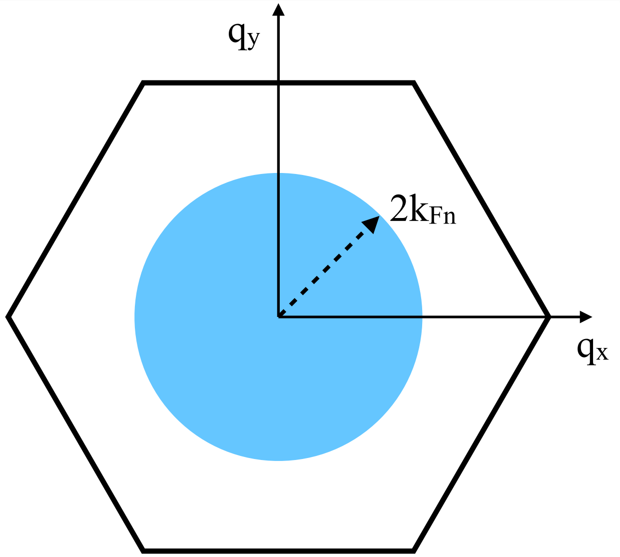


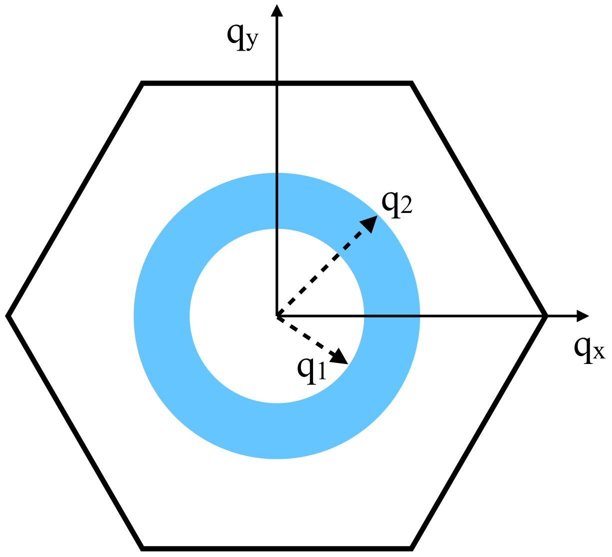


	λ_Γ	λ_K	λ_{TOT}	ω_{log} (meV)
Wannier (PBE)	0.095	0.053	0.148	74.27

Simplified superconductive model

Appl. Surf. Sci. 496, 143709 (2019)
arXiv:2001.08952 **[cond-mat.supr-con]**





$$\lambda = \sum_{\boldsymbol{q},\nu} \frac{N_{tot}(0)\langle g_\nu^2\rangle_{\boldsymbol{q}}}{\omega_{\boldsymbol{q}\nu}}$$

$$\log\{\omega_{log}\} = \frac{N_{tot}(0)}{2\lambda} \sum_{\boldsymbol{q},\nu} \frac{\langle g_\nu^2\rangle_{\boldsymbol{q}}}{\omega_{\boldsymbol{q}\nu}} \log\{\omega_{\boldsymbol{q}\nu}\}$$

$$|\boldsymbol{q}| = \sqrt{k_{Fn}^2 + k_{Fm}^2 - 2k_{Fn}k_{Fm}\cos\theta}$$

McMillan/Allen-Dynes:

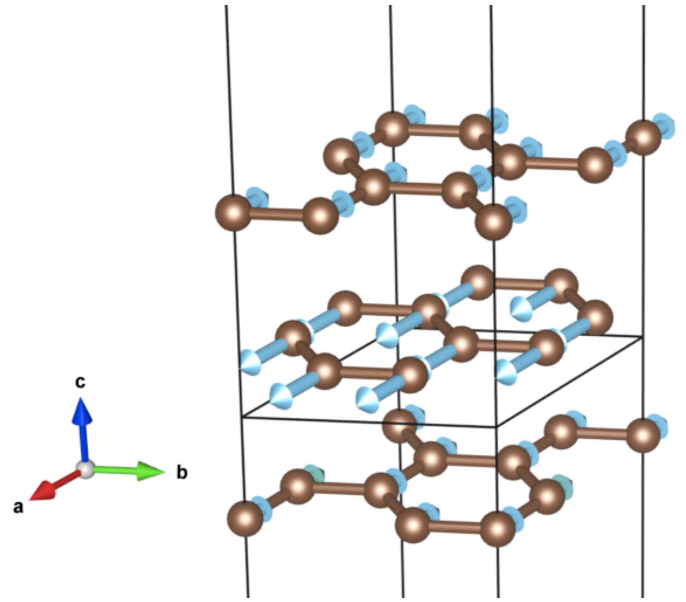
$$T_c = \frac{\omega_{log}}{1.2} exp\left\{-\frac{1.04(1+\lambda)}{\lambda - \mu^*(1+0.62\lambda)}\right\}$$

	λ_Γ	λ_K	λ_{TOT}	ω_{log} (meV)
Wannier (PBE)	0.095	0.053	0.148	74.27
Simple PBE	0.096	0.012	0.108	113

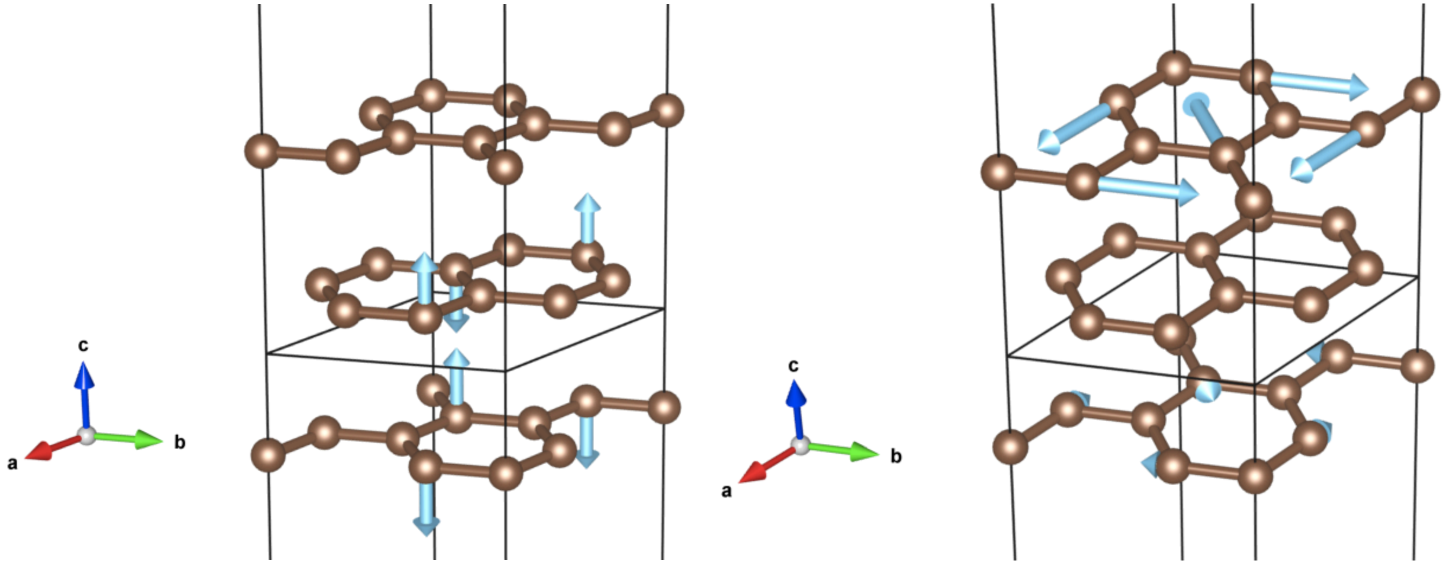
- The simplified model slightly underestimates the Wannier-interpolated values;
- In both cases, no superconductivity is found ($\boldsymbol{\mu}^*$=0.1).

Simplified superconductive model

q=Γ



q=K



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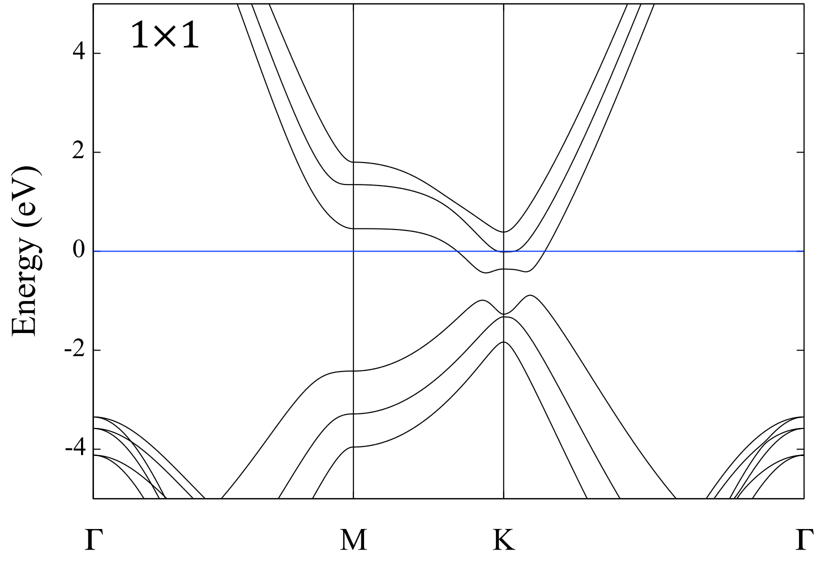
Finite differences computation of e-ph matrix elements

C. Attaccalite, Phys. Status Solidi B 246, No. 11–12, 2523–2526 (2009)



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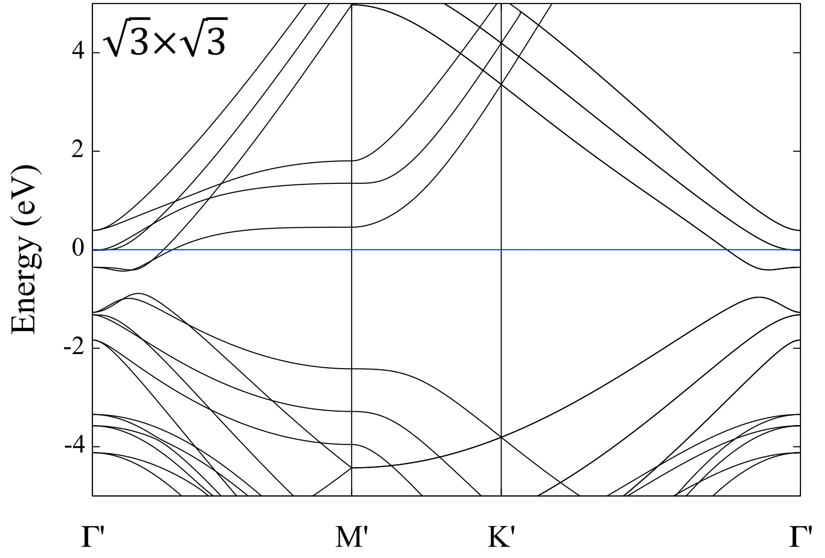

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- **The electron-phonon matrix elements are proportional to the variations of the KS Hamiltonian with respect to atom displacement**:

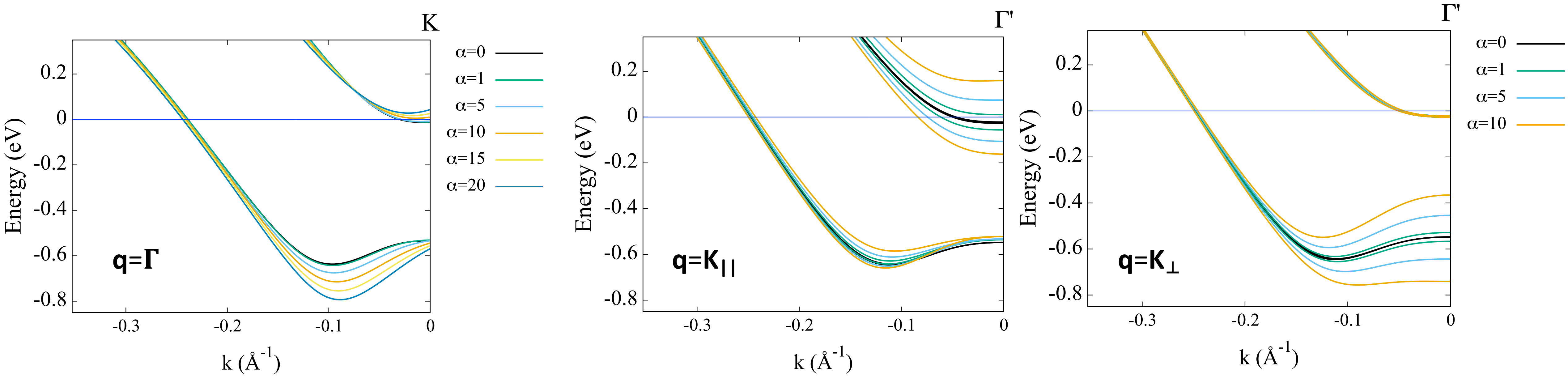
$$g^{\nu}_{\boldsymbol{K}n,\boldsymbol{K}+\boldsymbol{q}m} \propto \left\langle \phi_n \left| \frac{\delta H_{KS}}{\delta \boldsymbol{u}^{\nu}_{\boldsymbol{q}}} \right| \phi_m \right\rangle = \left\langle \phi_n \left| \frac{H_{KS}\left(\alpha \boldsymbol{u}^{\nu}_{\boldsymbol{q}}\right) - H_{KS}(0)}{\left|\boldsymbol{u}^{\nu}_{\boldsymbol{q}}\right|} \right| \phi_m \right\rangle$$

- We need to calculate the variation of the eigenvalue (i.e. the electronic band) as a function of an atomic displacement.

- This technique requires the knowledge of the phonon displacement for the modes giving rise to strong electron-phonon interactions;

- Notice that, in order to obtain the correct phonon displacement, the **q=K** mode will be computed in a $\sqrt{3}\times\sqrt{3}$ supercell, where **K** is folded into **Γ**

Electron-phonon boost via hybrid functionals



	λ_Γ	λ_K	λ_{TOT}
Simple PBE	0.096	0.012	0.108
Simple PBE0	0.218	0.028	0.246
Simple B3LYP	0.197	0.035	0.232

Conclusions

- A simplified superconductive model correctly describes the system under study from a qualitative point of view, slightly underestimating λ;
- The inclusion of the exact exchange interaction among electrons via hybrid functionals boost the electron-phonon coupling constant λ by approximately a factor 2;
- The McMillan/Allen-Dynes formula (μ^*=0.1), together with the computed values of λ and ω_{log}, shows that phonon mediated superconductivity is not induced in such system for $n_{2D}<2\cdot10^{14}$ cm^{-2}.

Thank you for your attention!

Acknowledgments

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