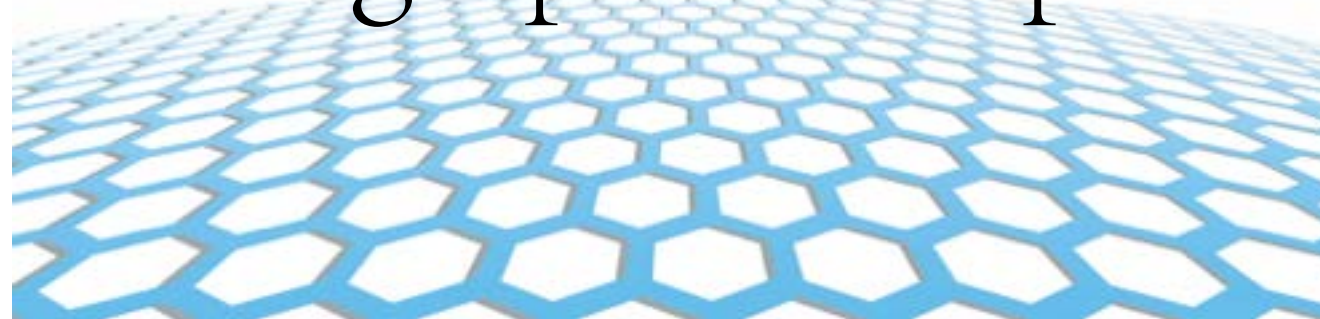




How to make graphene superconducting



Gianni Profeta

Physics Department, University of L'Aquila, Italy

&

Max-Planck Institute of Microstructure Physics, Halle, Germany

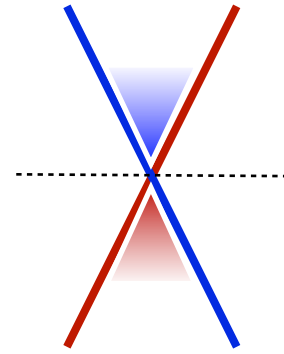
Matteo Calandra and Francesco Mauri

IMPMC, University of Paris 6, CNRS, Jussieu, Paris France

Graphene: physical realization of fundamental phenomena in solid-state-physics

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- Ultra-relativistic particles near E_F $E = \pm v_F \mathbf{p}$, $v_F = c/300$



A. H. Castro Neto et al. RMP (2009)

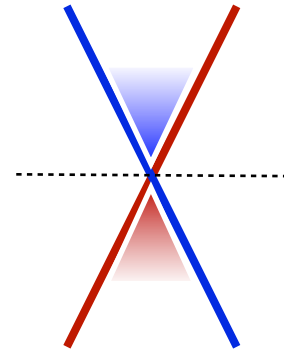
Novoselov et al. Nature (2005)

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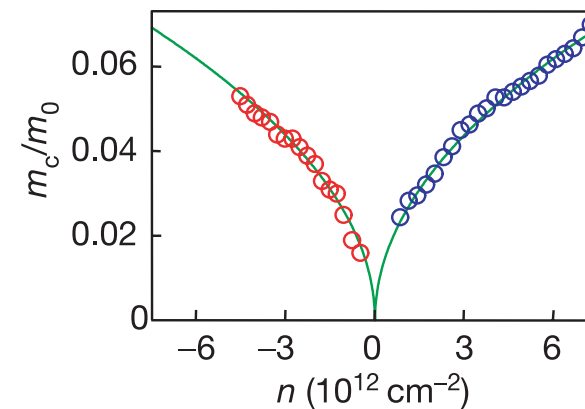
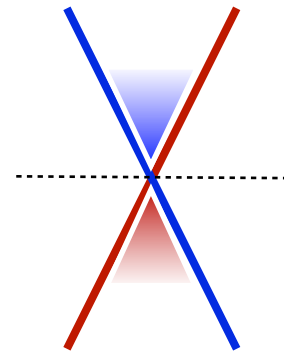
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- Cyclotron mass with carriers

$$m_c \propto \sqrt{n}$$



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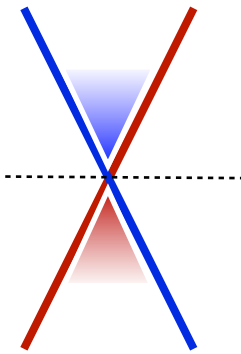
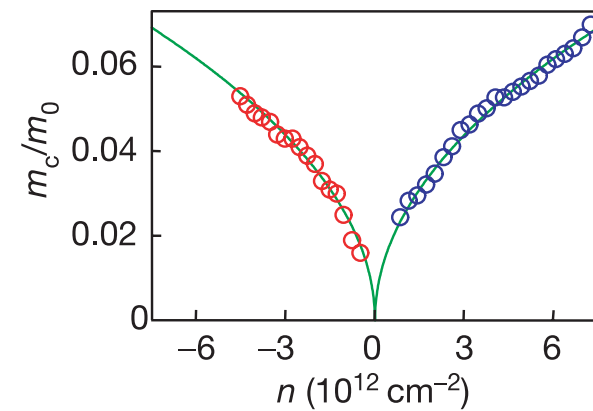
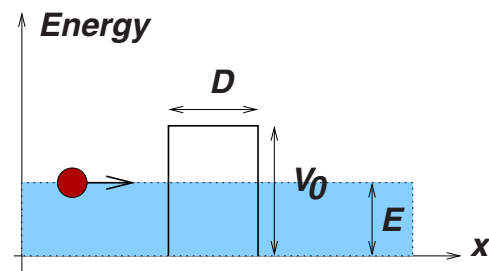
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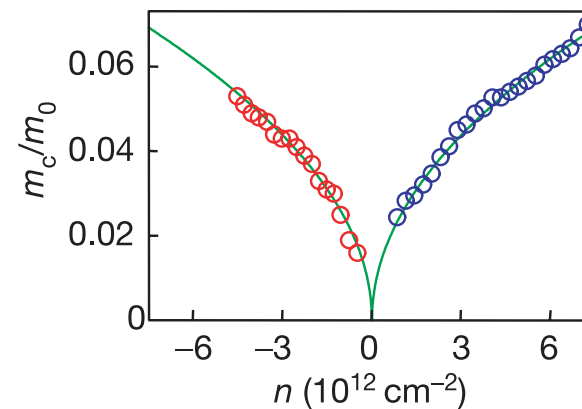
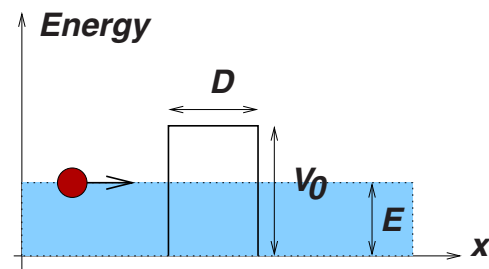
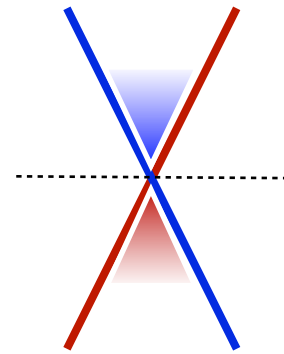
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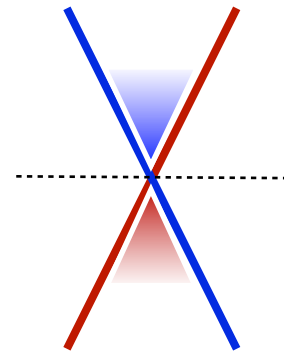
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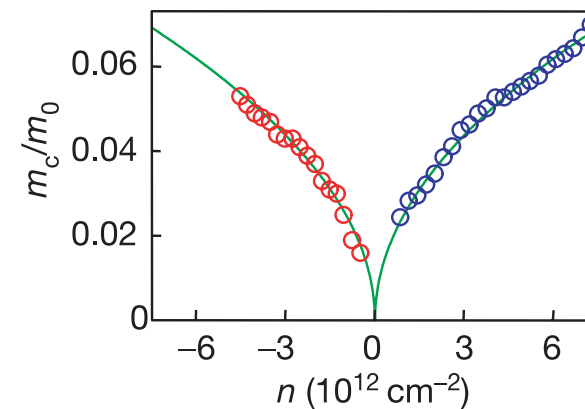
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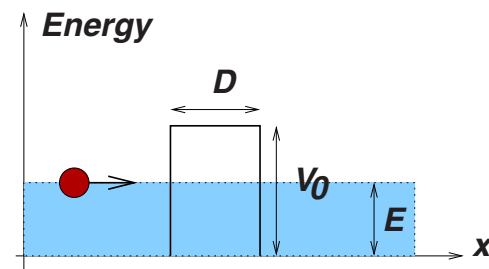


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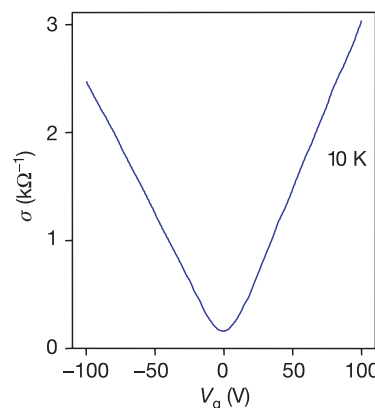
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- High stiffness and high mobility



- Ambipolar



A. H. Castro Neto et al. RMP (2009)

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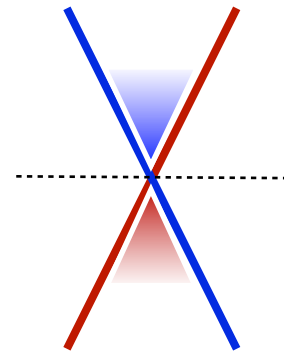
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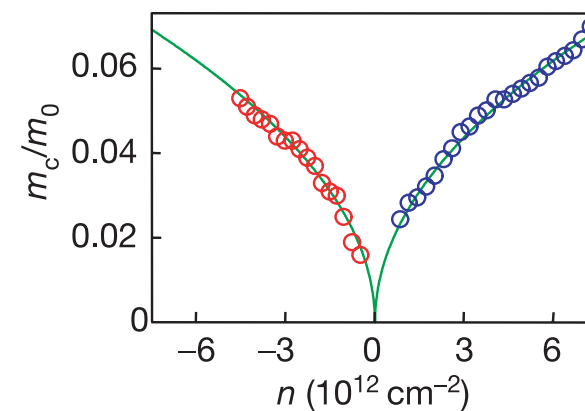
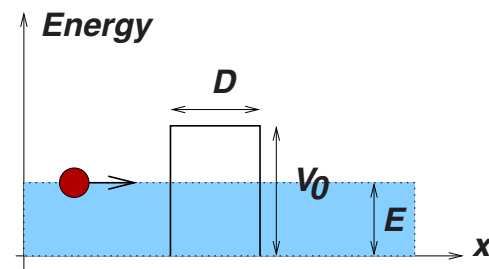
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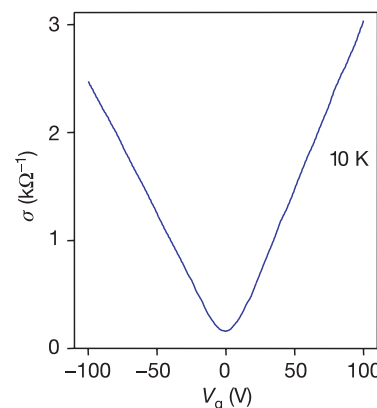
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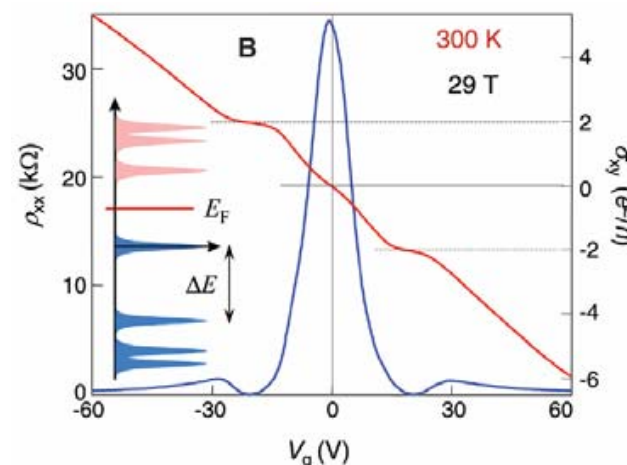
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...but in the long list of graphene remarkable properties, a fundamental block is missing:

SUPERCONDUCTIVITY

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Some experimental discoveries

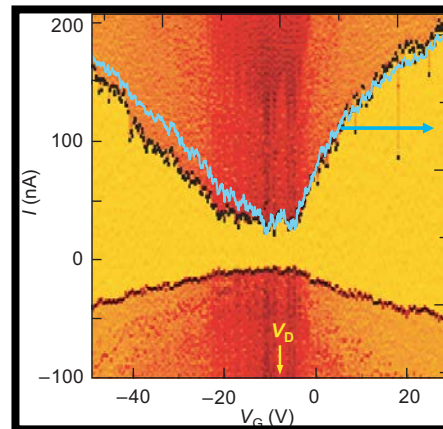
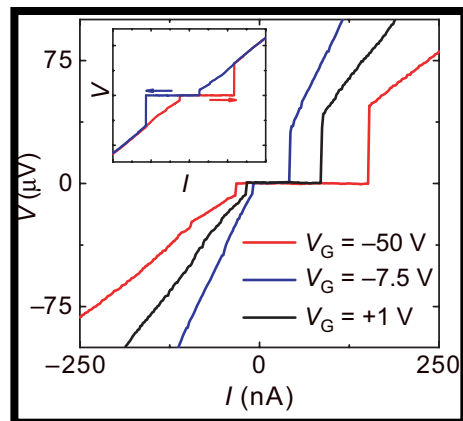
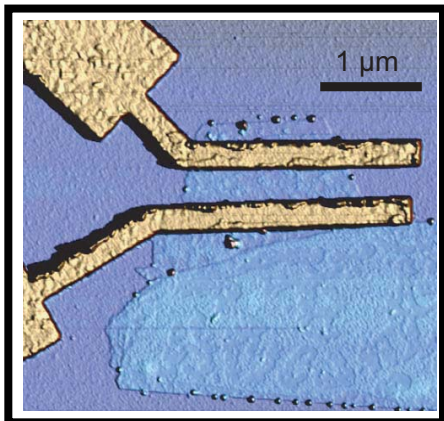
nature

Vol 446 | 1 March 2007 | doi:10.1038/nature05555

LETTERS

Bipolar supercurrent in graphene

Hubert B. Heersche^{1*}, Pablo Jarillo-Herrero^{1*}, Jeroen B. Oostinga¹, Lieven M. K. Vandersypen¹
& Alberto F. Morpurgo¹



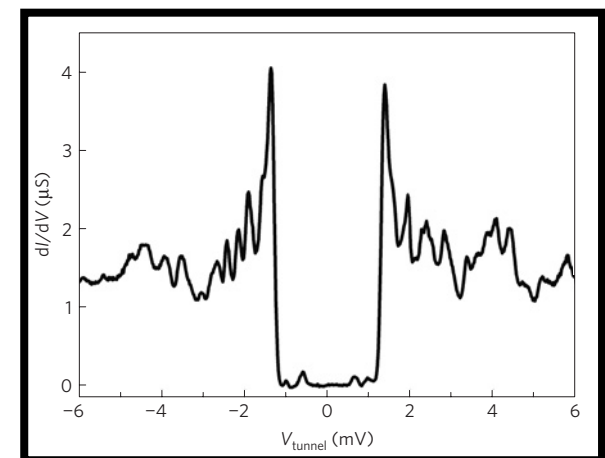
LETTERS

PUBLISHED ONLINE: 6 FEBRUARY 2011 | DOI: 10.1038/NPHYS1911

nature
physics

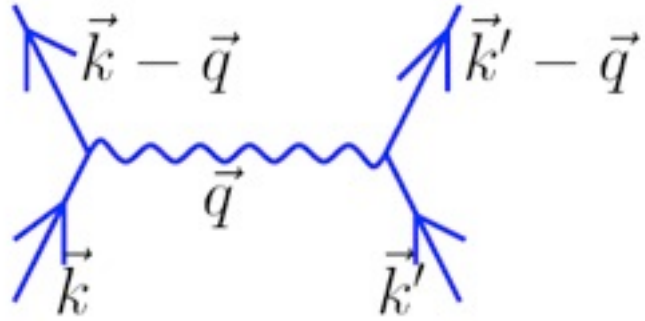
Transport through Andreev bound states in a graphene quantum dot

Travis Dirks, Taylor L. Hughes, Siddhartha Lal[†], Bruno Uchoa, Yung-Fu Chen, Cesar Chialvo, Paul M. Goldbart[†] and Nadya Mason^{*}



Superconductivity: Is it expected?

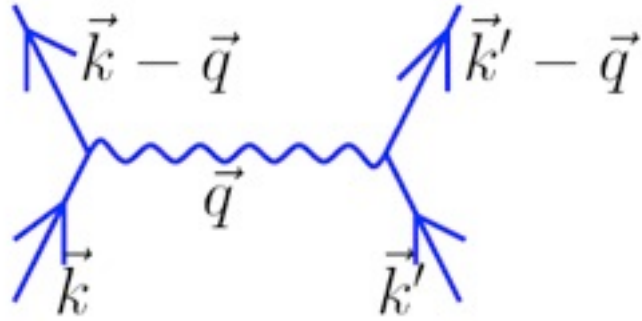
Superconductivity: Is it expected?



The total electron-phonon coupling is :

$$\lambda = \frac{N(0)D^2}{M\omega^2}$$

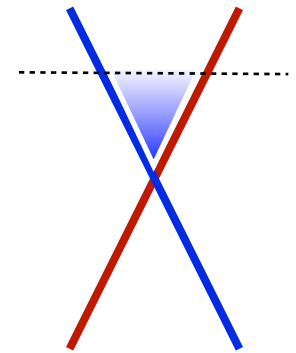
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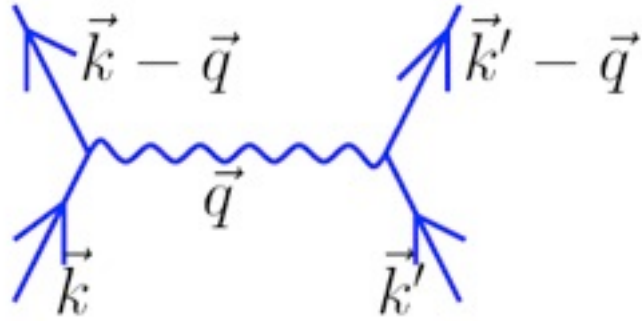
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$N(0)$ is vanishingly small, however it can be varied by rigid doping
but it increases very slowly



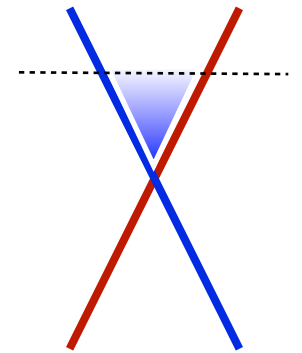
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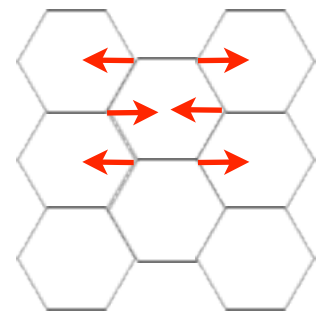
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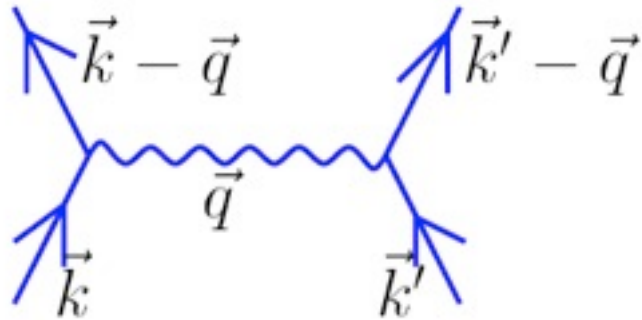
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The deformation potential, D , for in-plane modes is high, but $1/\omega^2$ is low



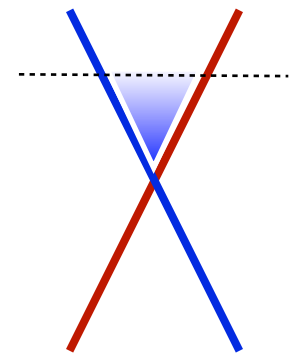
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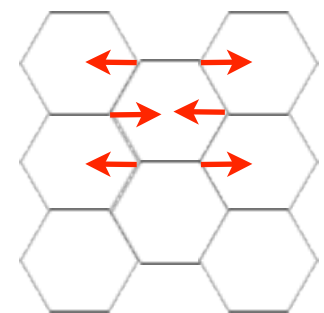
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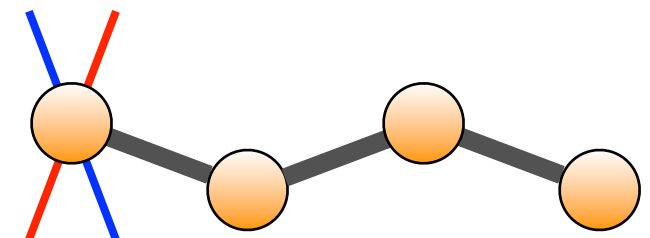
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By symmetry out-of-plane modes do not couple with π electrons



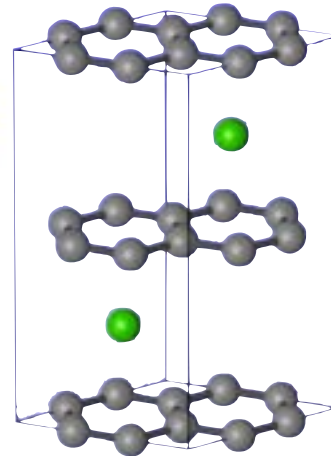
Superconductivity in Graphite

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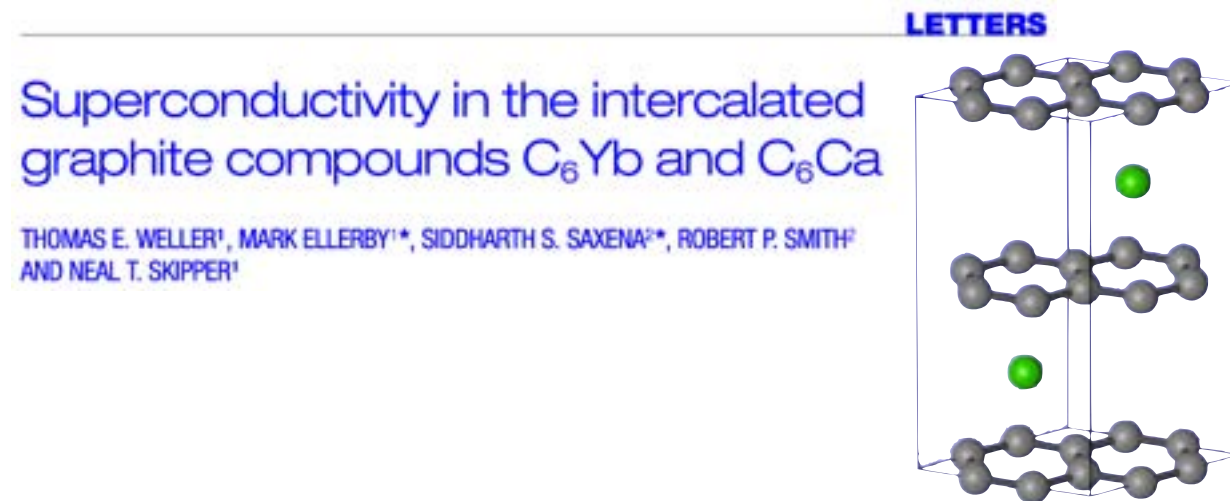
LETTERS

Superconductivity in the intercalated
graphite compounds C_6Yb and C_6Ca

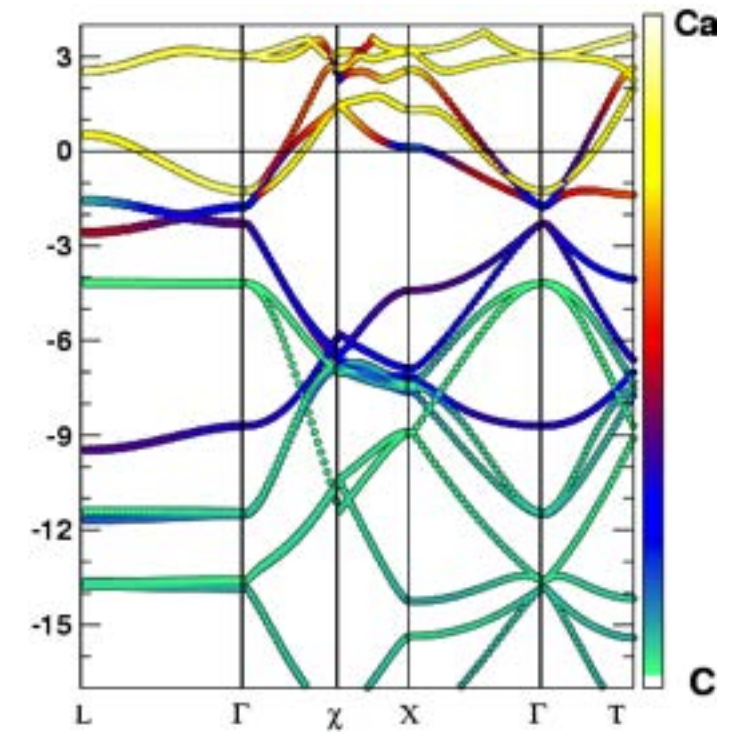
THOMAS E. WELLER¹, MARK ELLERBY^{1*}, SIDDHARTH S. SAXENA^{2*}, ROBERT P. SMITH²
AND NEAL T. SKIPPER¹



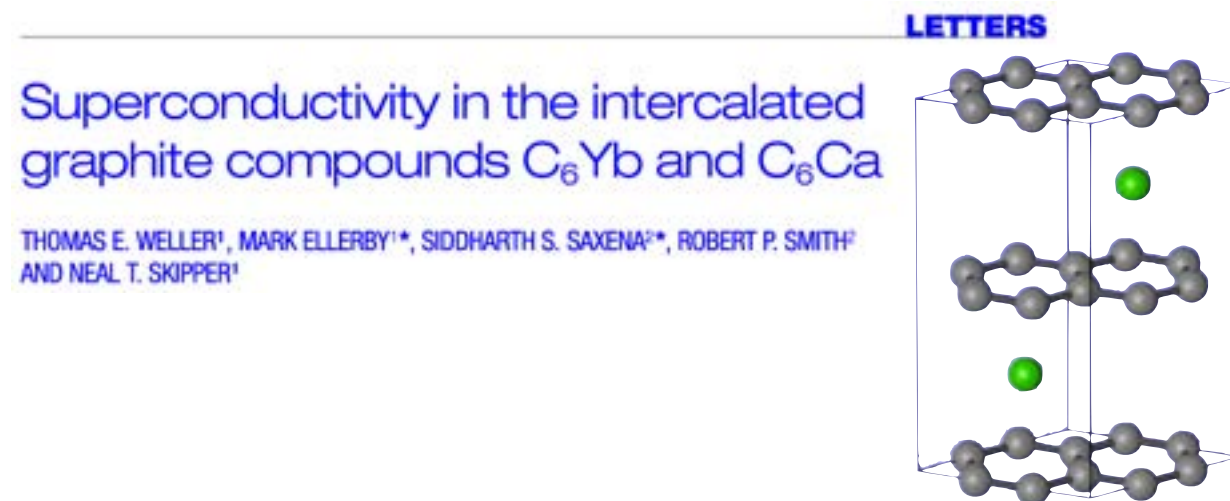
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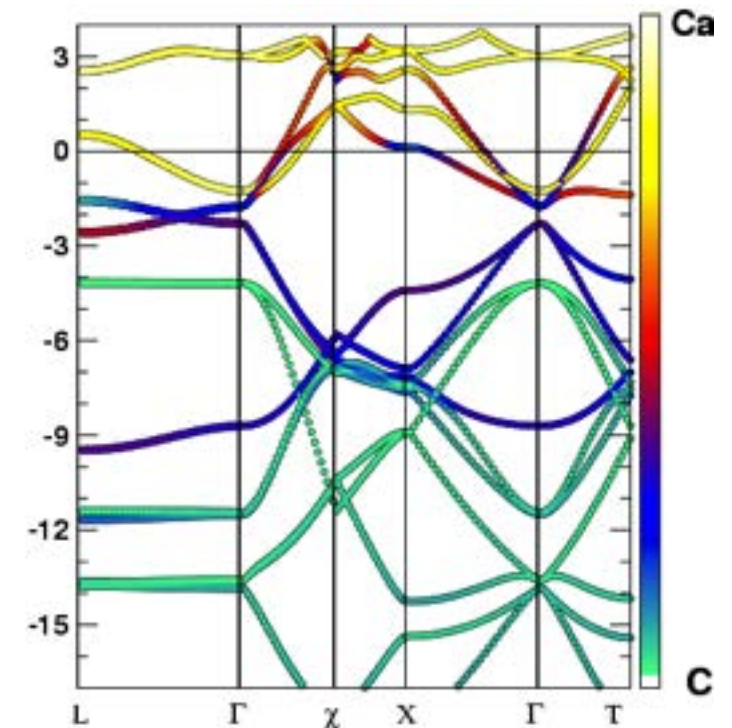
The interlayer state



Superconductivity in Graphite

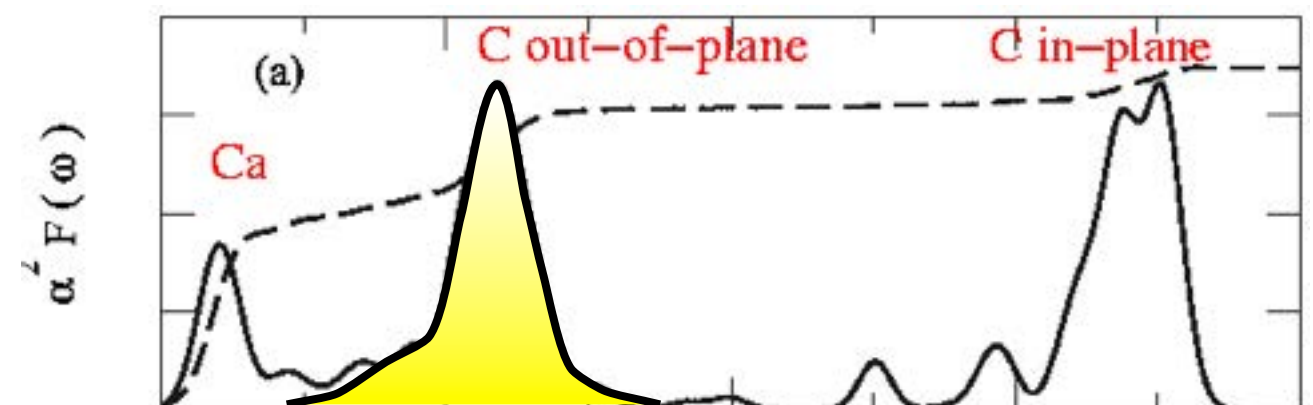


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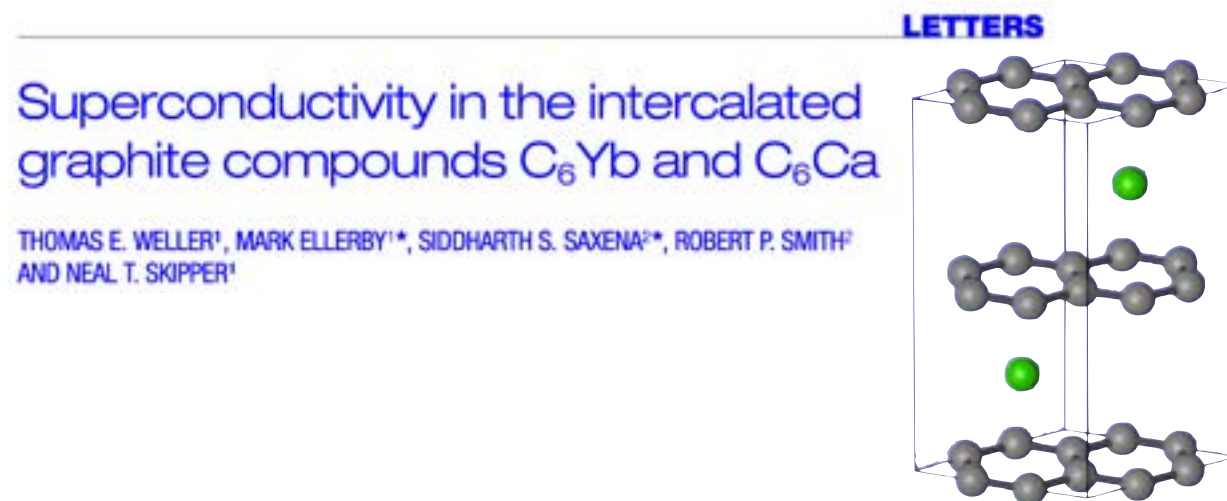


The electron-phonon coupling:
 C_z coupling

M. Calandra and F. Mauri, Phys. Rev. Lett (2005)



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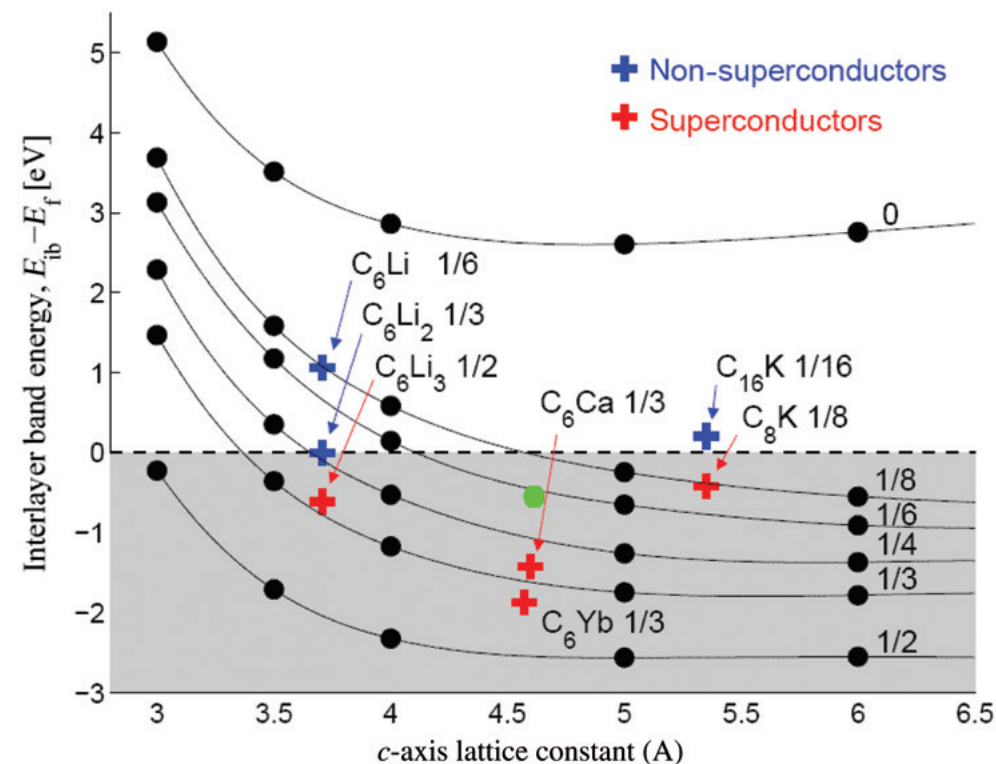


The Cambridge criterion

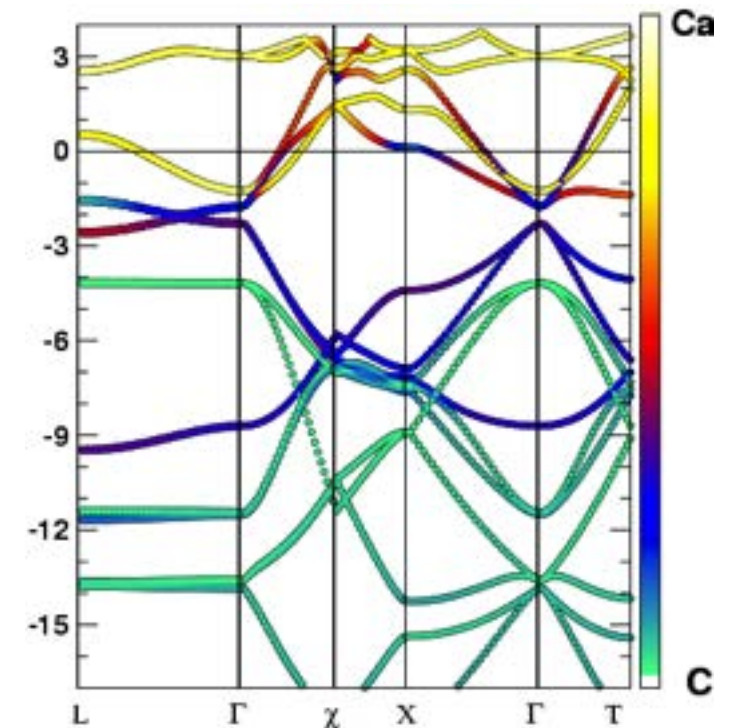
M. S. Dresselhaus and G. Dresselhaus, Adv. in Phys. (2002)

G. Csanyi et al, Nat. Phys. (2005)

I. Mazin and A. V. Balatsky Phil. Mag. Lett. (2010)

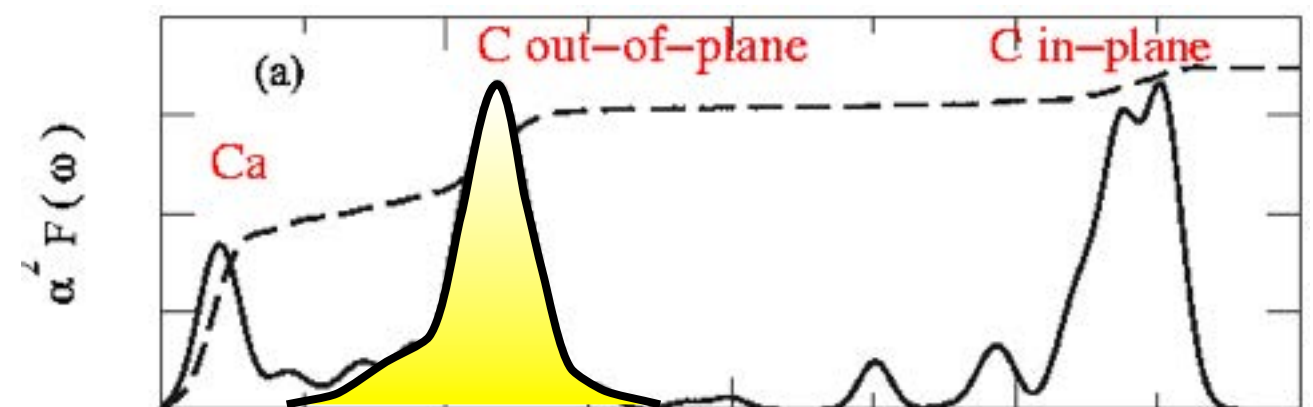


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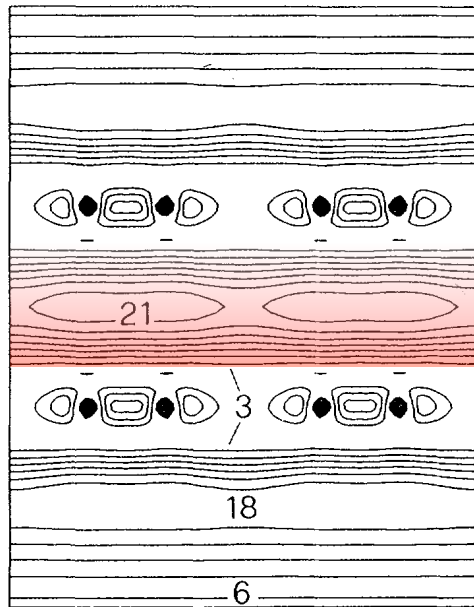


The electron-phonon coupling: C_z coupling

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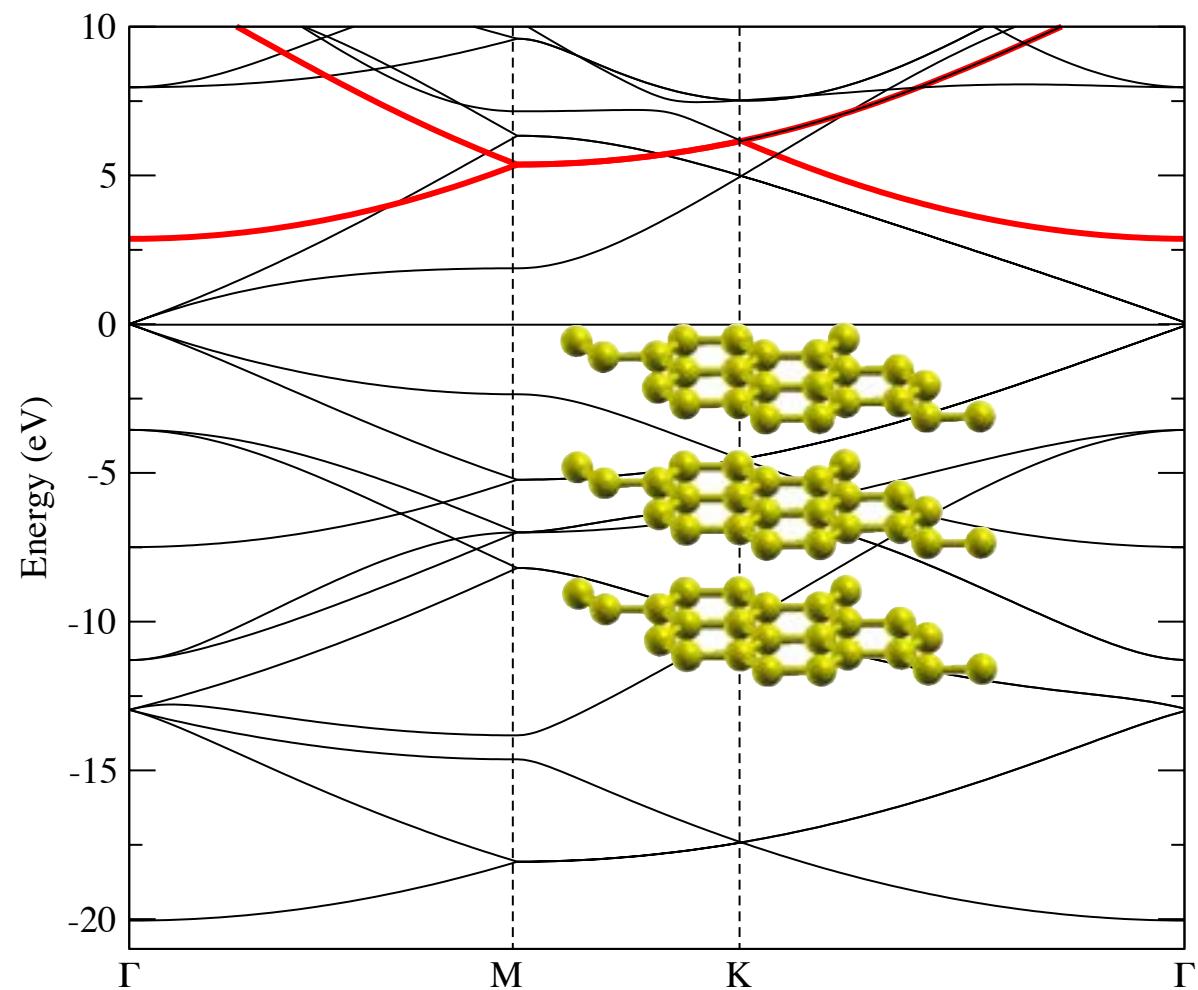
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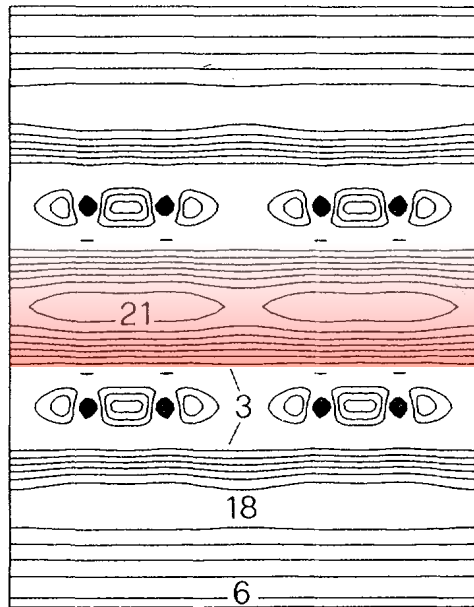
It is a strongly 3D dispersive state living between carbon layers*

* *M. Posternak et al. Phys. Rev. Lett. (1983)*

L. Boeri et al. Phys. Rev. B (2007)



The interlayer state



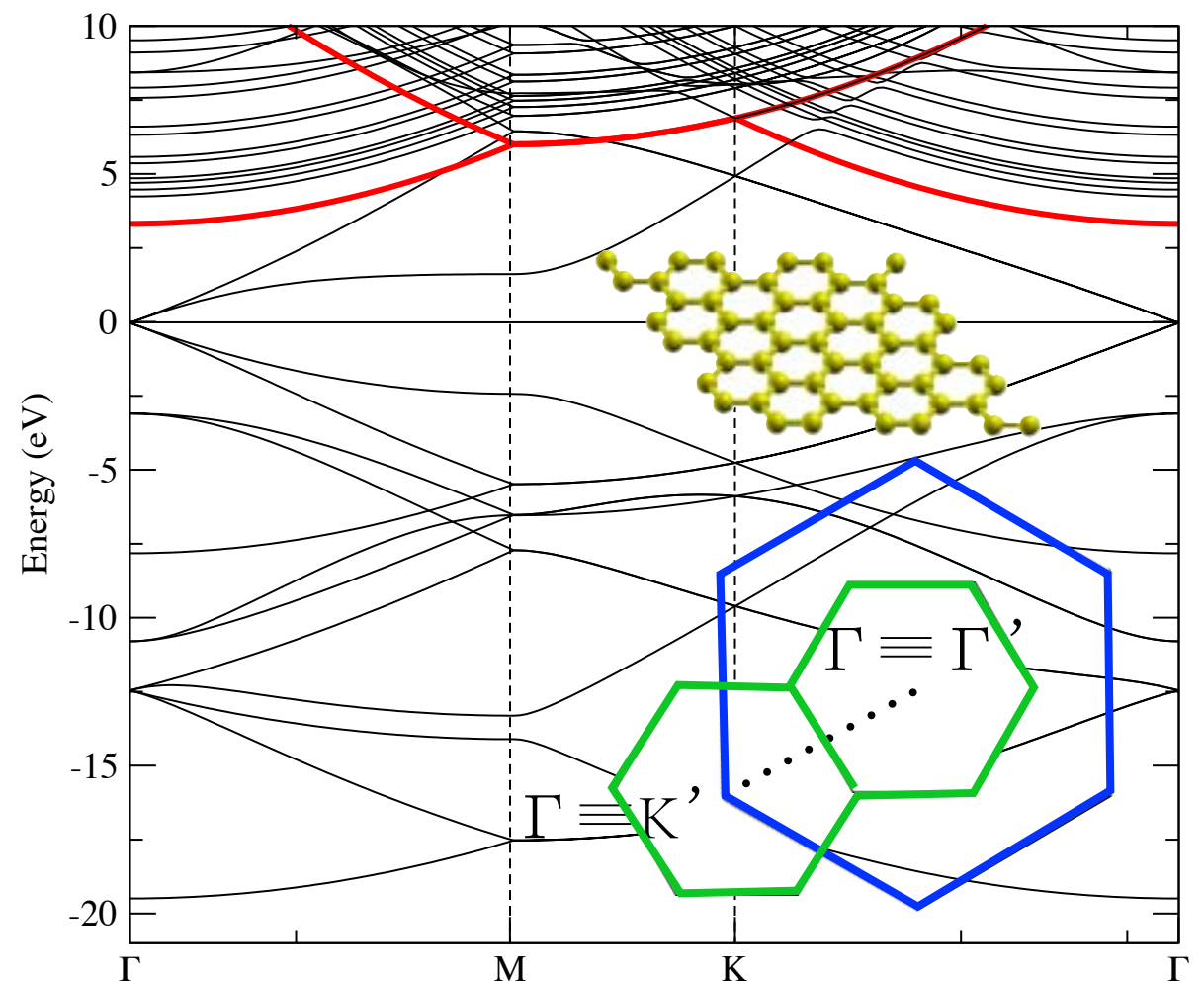
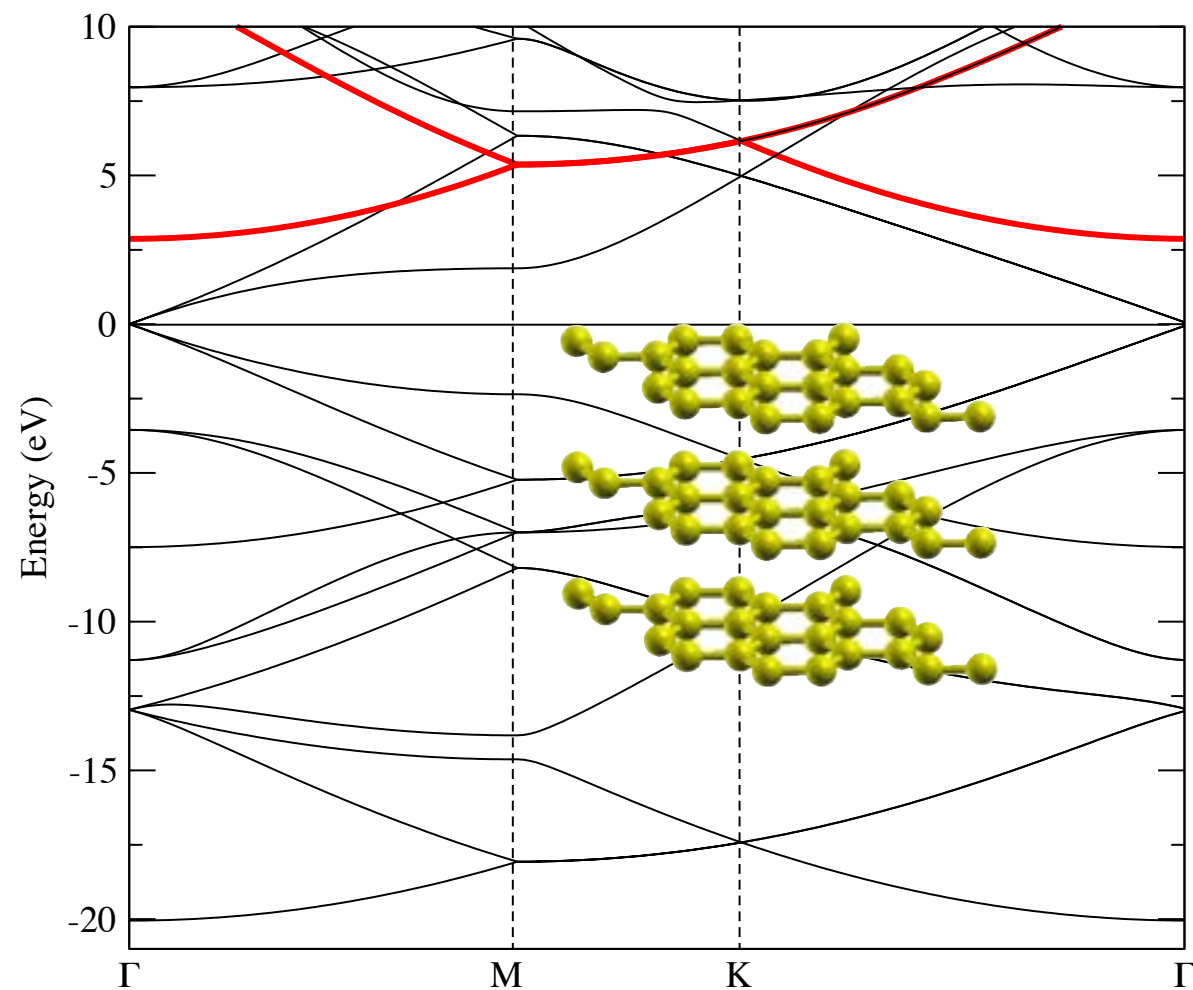
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L. Boeri et al. Phys. Rev. B (2007)

But it exists even in multiwall nanotubes, fullerenes, BN, MgB₂ and.....

.....graphene

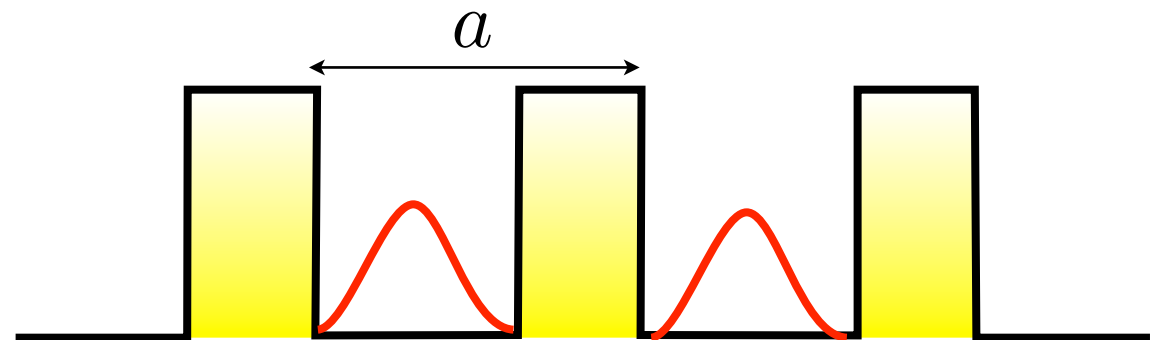
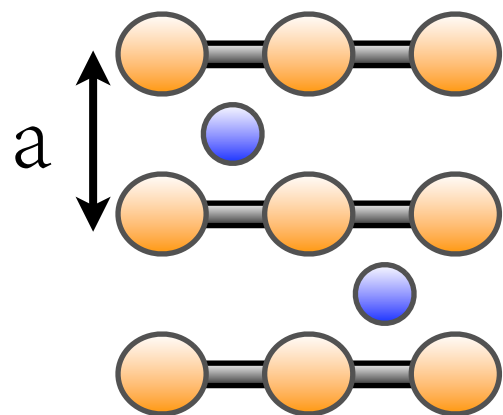


Use the interlayer state: put it at E_F

Interlayer state is a truly 2D free-electron state in xy direction, $\psi(x, y) = e^{i(k_x x + k_y y)}$

However, in the z direction is not exactly “free” .

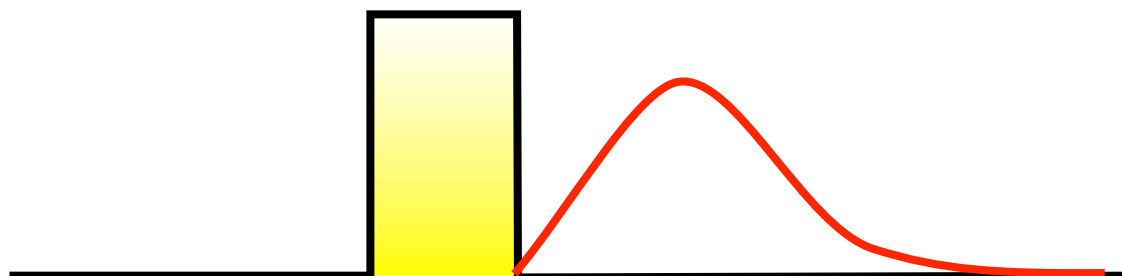
Kronig-Penney model of bulk GIC



$$E_n = n^2 \frac{\hbar^2}{2m} \frac{\pi^2}{a^2}$$

The interlayer state energy decreases removing the quantum confinement along z

$$a \rightarrow \infty$$



that is Metal adatoms on Graphene

Metal doped Graphene

We performed first-principles Density Functional Theory calculation of structural, electronic, dynamical and superconducting properties of metal adatoms on Graphene

The electron-phonon matrix element

$$g_{nm}^{\nu}(\mathbf{k}, \mathbf{k} + \mathbf{q}) \propto \langle \mathbf{k} + \mathbf{q}m | \frac{\delta v_{\text{SCF}}}{\delta \mathbf{u}_{\mathbf{q}s}} | \mathbf{k}n \rangle$$

Phonon linewidth

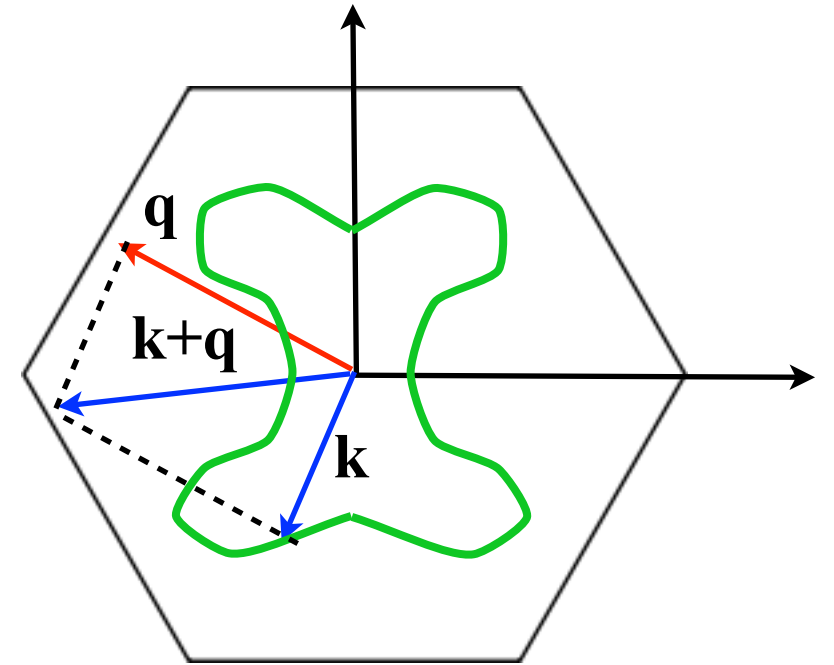
$$\gamma_{\mathbf{q}\nu} = \frac{4\pi\omega_{\mathbf{q}\nu}}{N_k(T)} \sum_{\mathbf{k}, n, m}^{N_k(T)} |g_{nm}^{\nu}(\mathbf{k}, \mathbf{k} + \mathbf{q})|^2 \delta(\varepsilon_{\mathbf{k}n}) \delta(\varepsilon_{\mathbf{k}+\mathbf{q}m})$$

$$\lambda_{\mathbf{q}\nu} = \frac{\gamma_{\mathbf{q}\nu}}{2\pi\omega_{\mathbf{q}\nu}^2 \mathcal{N}_s}$$

The Eliashberg function

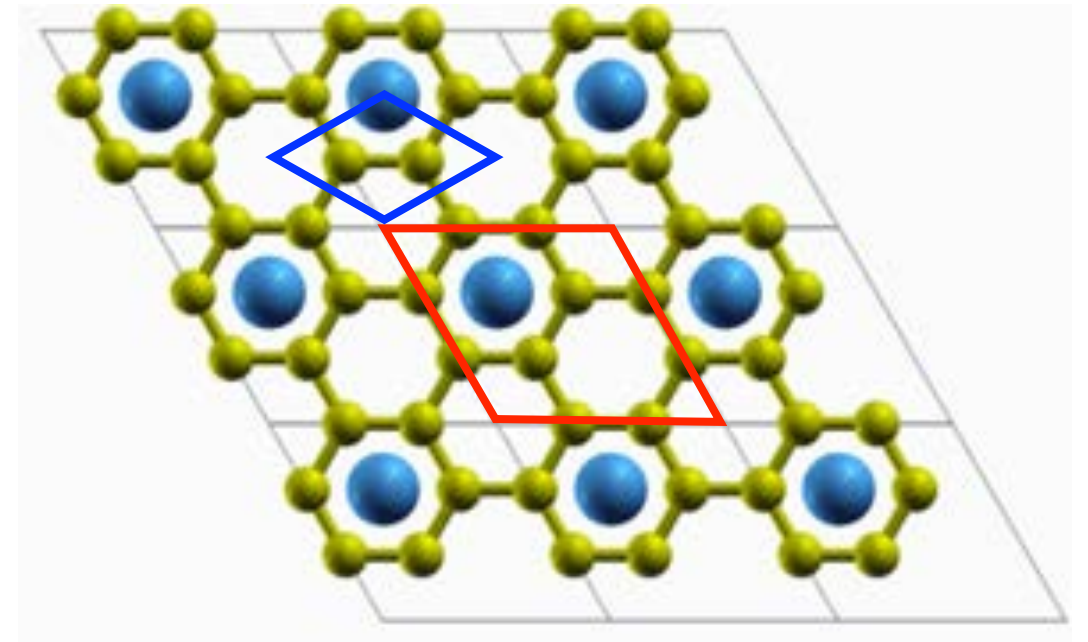
$$\alpha^2 F(\omega) = \frac{1}{2N_q} \sum_{\mathbf{q}\nu} \lambda_{\mathbf{q}\nu} \omega_{\mathbf{q}\nu} \delta(\omega - \omega_{\mathbf{q}\nu})$$

$$T_c = \frac{\omega_{log}}{1.20} \exp\left\{-\frac{1.04(1+\lambda)}{\lambda - \mu^*(1+0.62\lambda)}\right\}$$



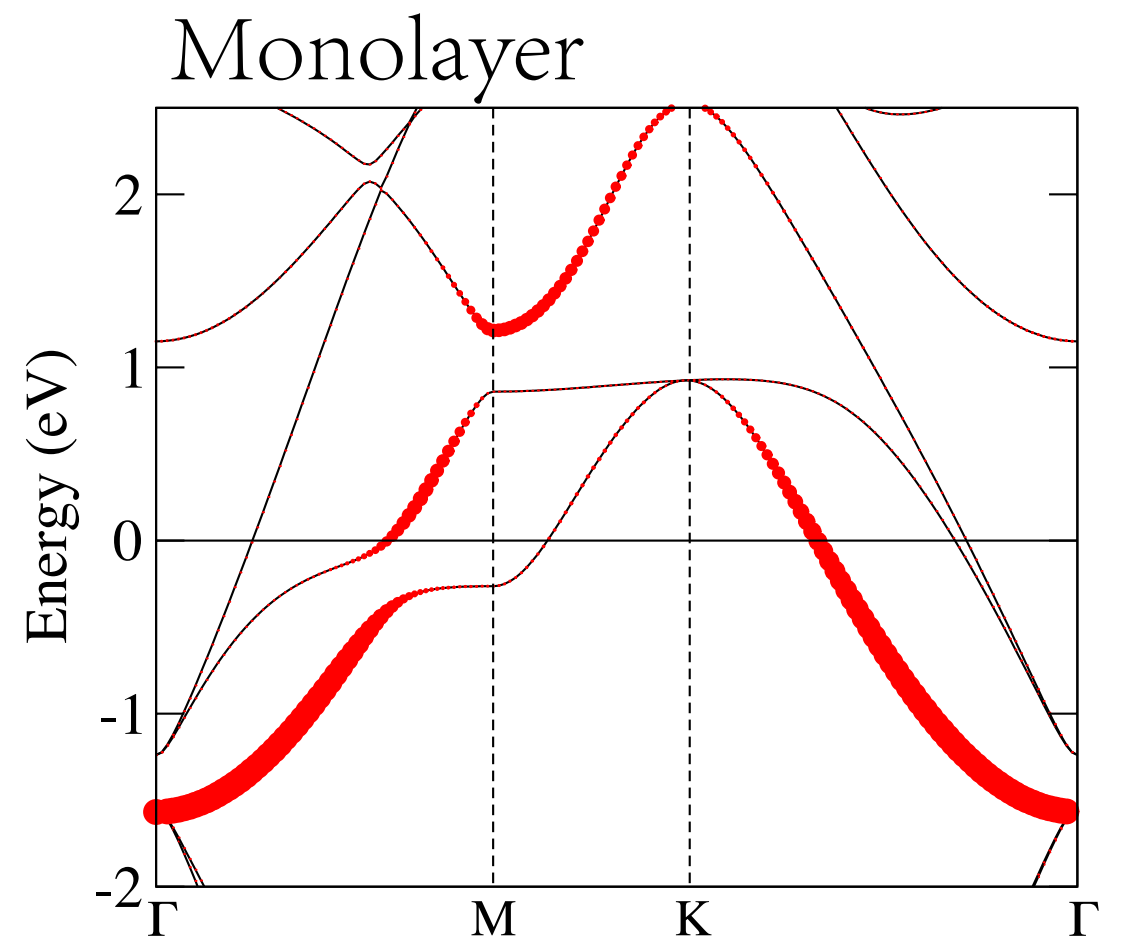
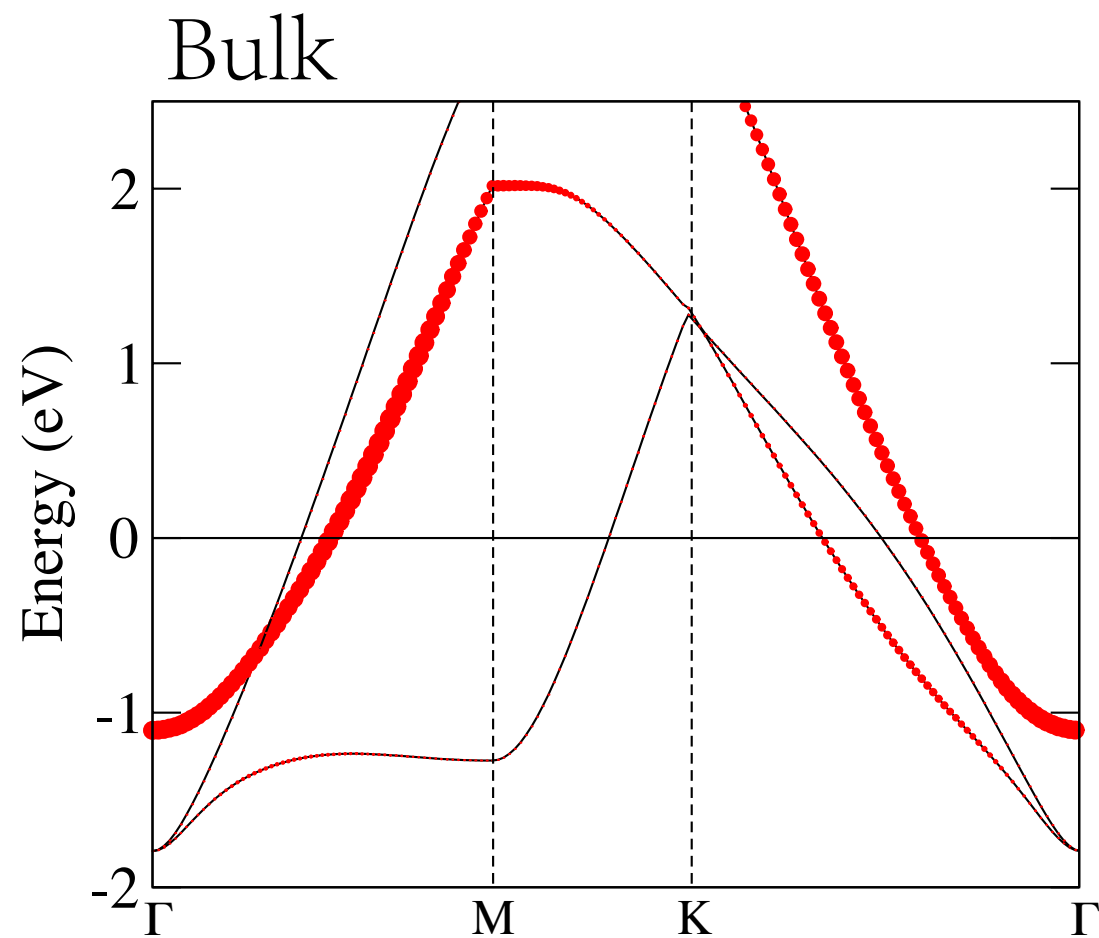
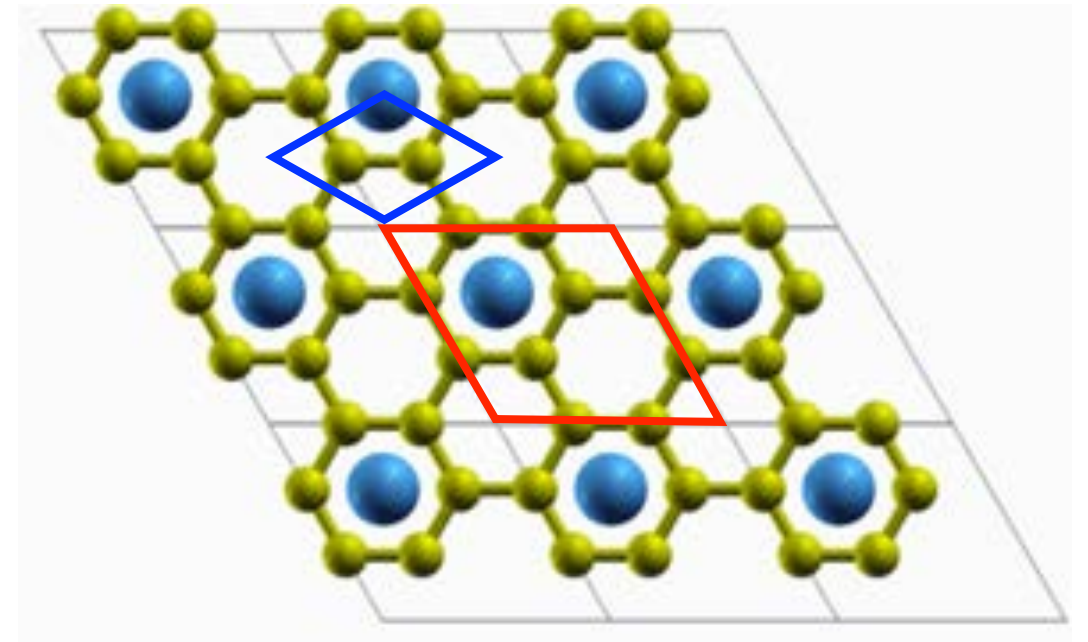
Metal doped Graphene

- Ca is the first choice (CaC_6 has $T_c=11.5\text{ K}$)
- Ca adsorbs in the hollow site at $2.24\text{ \AA}$
- IL at E_F ?

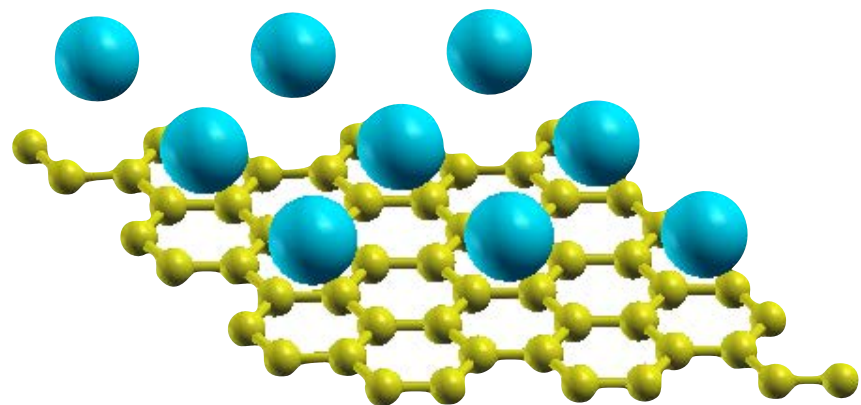
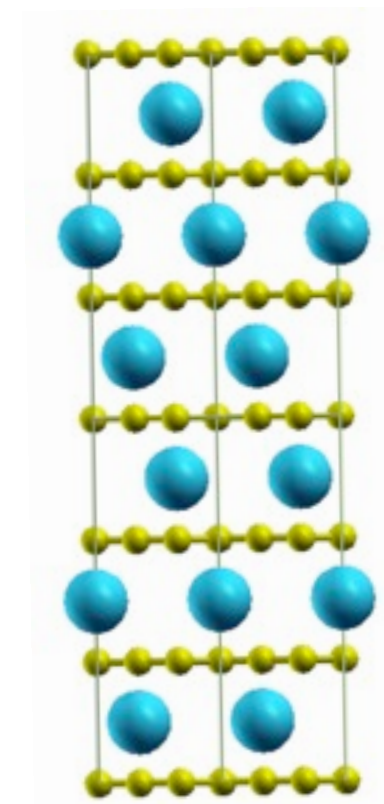
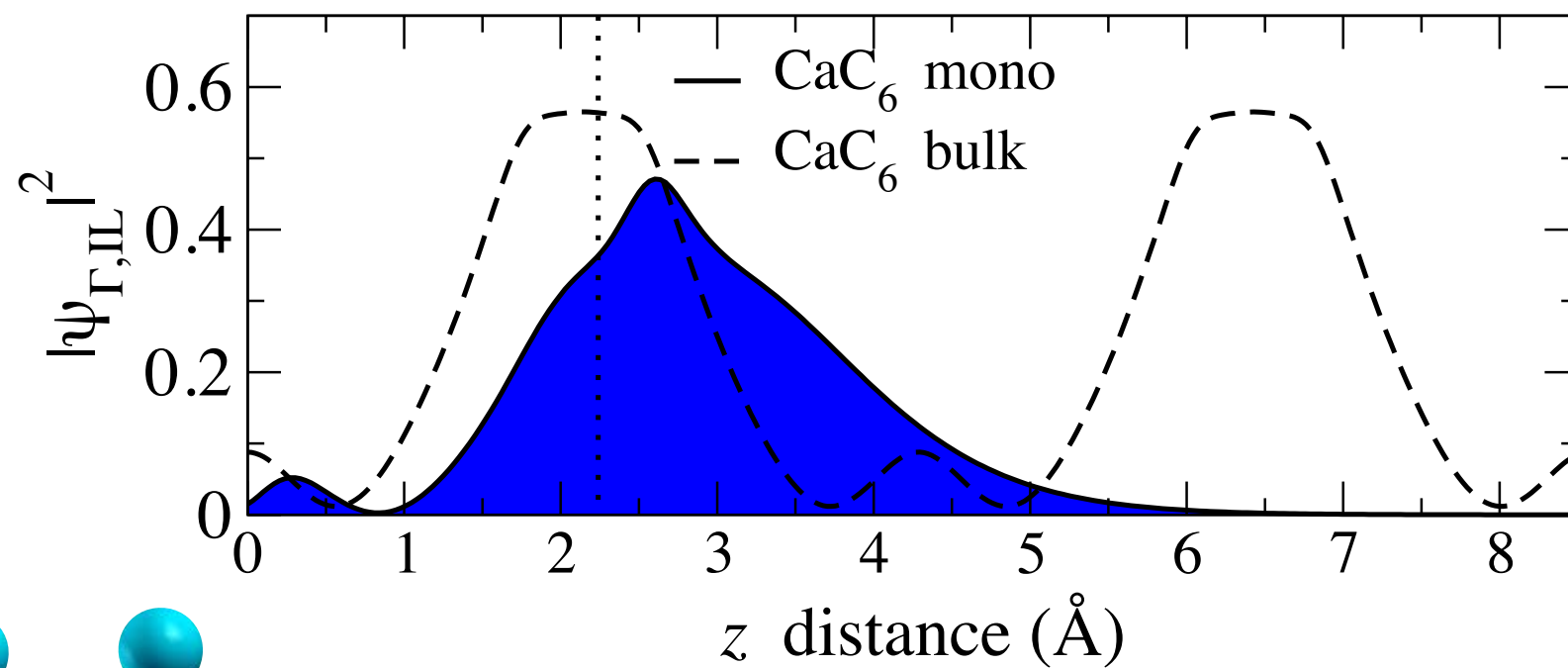


Metal doped Graphene

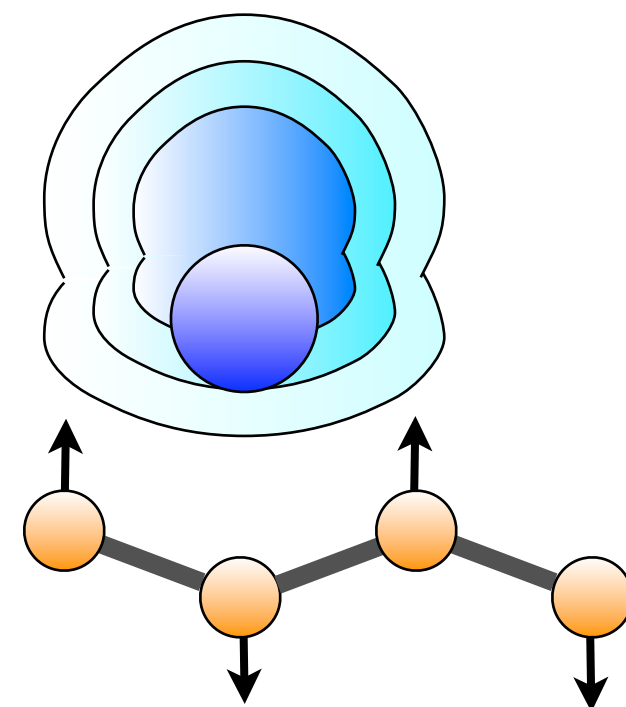
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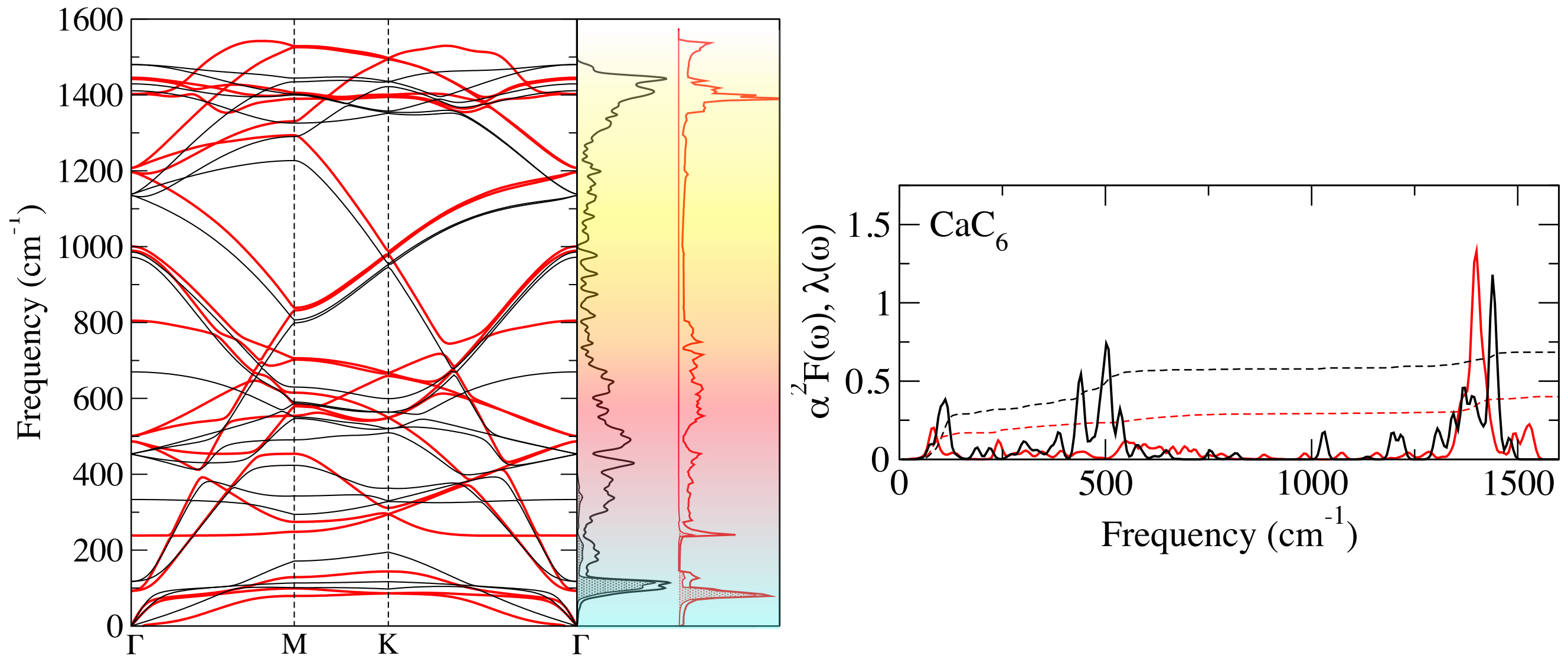
Ca on graphene: The interlayer state



The IL moves away from graphene, reducing the electron-phonon coupling with C_z modes



Ca on graphene: electron-phonon coupling



The coupling with C_z modes, present in the bulk compound, is small in the monolayer case

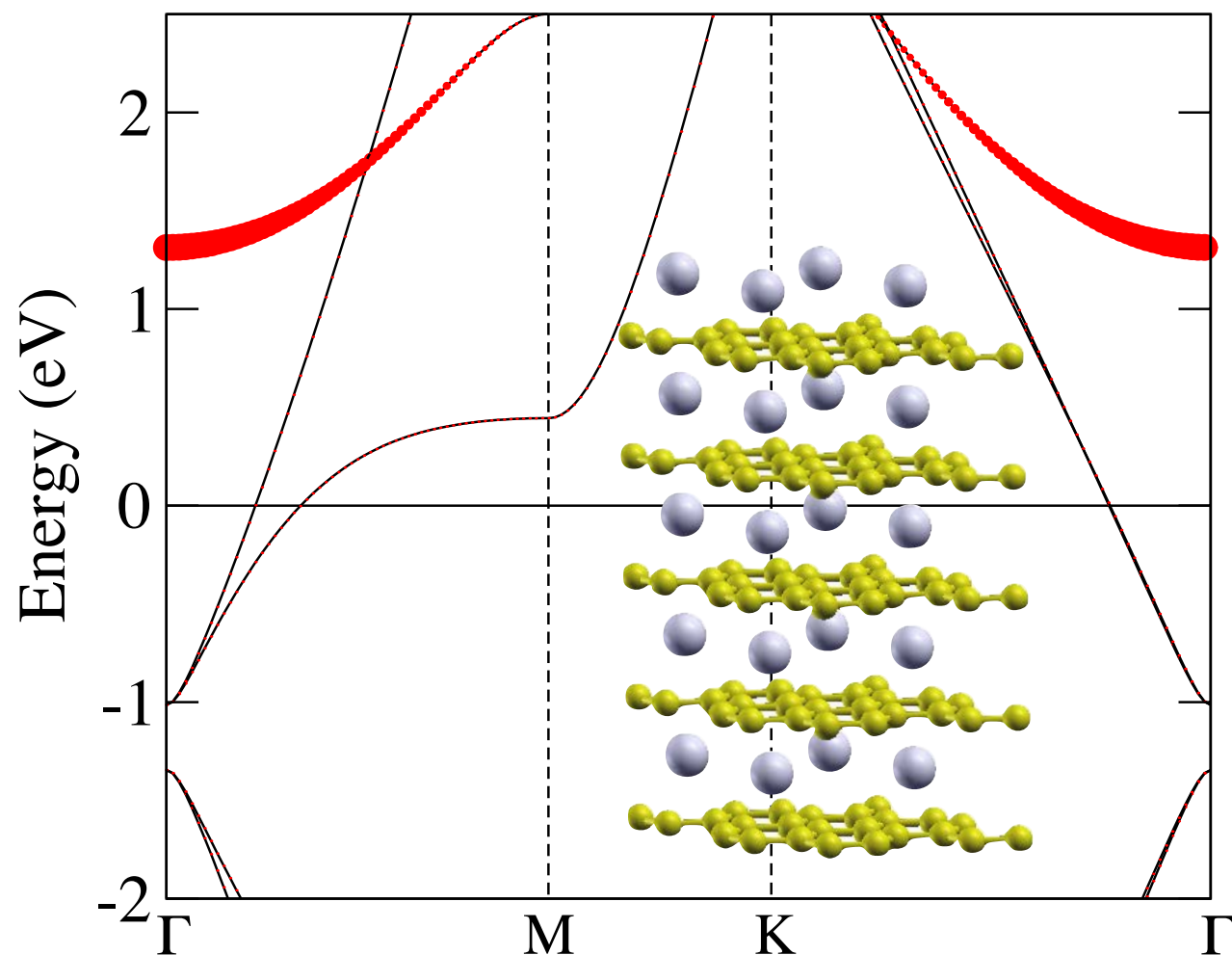
The total electron-phonon coupling is $\lambda = 0.40$ with an estimated $T_c = 1.4 \text{ K}$ ($\lambda = 0.70$ and $T_c = 11.5 \text{ K}$)

Removal of quantum confinement reduces λ : Bulk better than Film

Lithium doped Graphene

- There is at least one case among GICs that can be further explored, stage-1 Lithium GIC, LiC_6 .
- IL state is completely empty: the strong quantum confinement prevents its occupation
- It is not superconducting

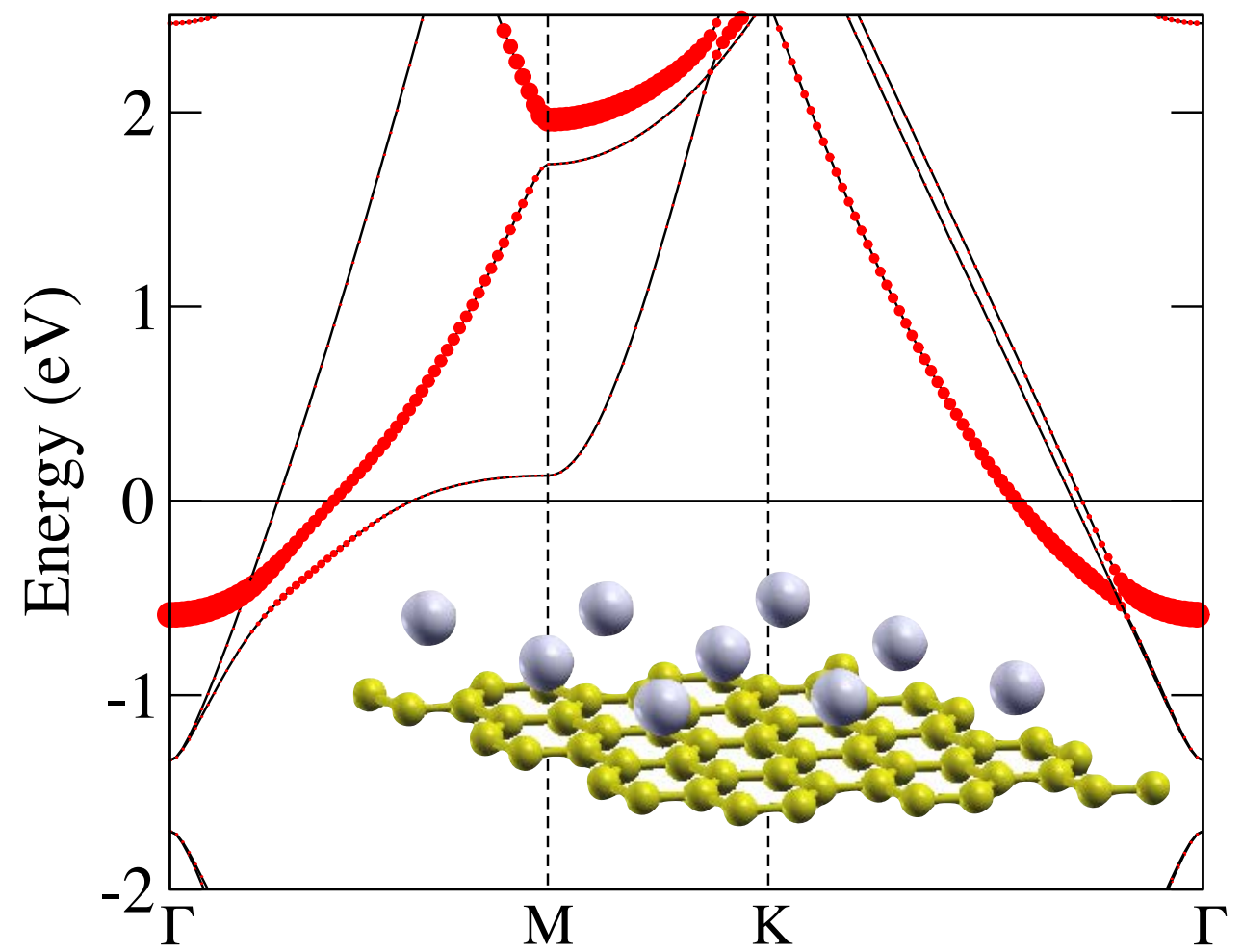
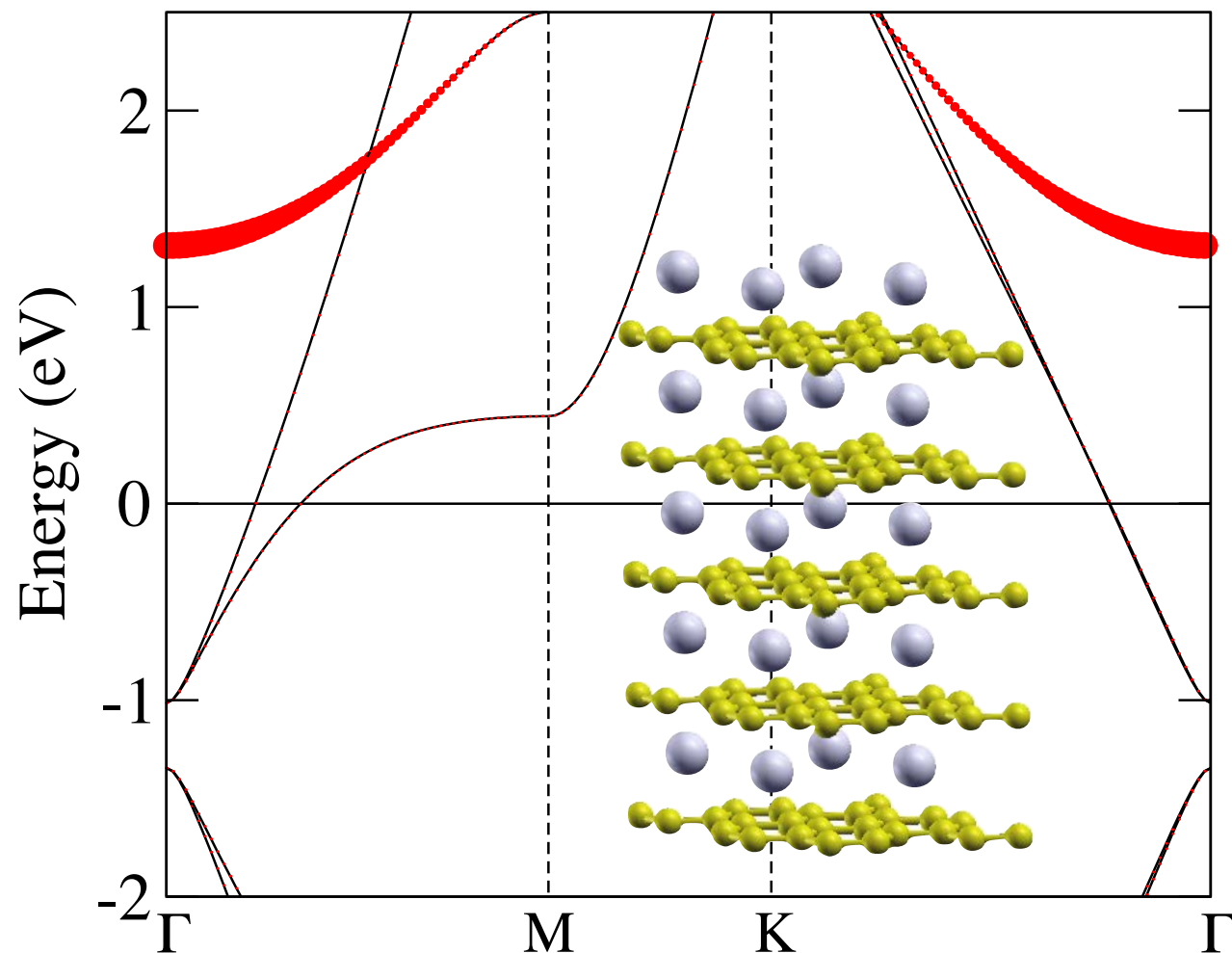
Removal of confinement along c direction should bring the IL at the Fermi level



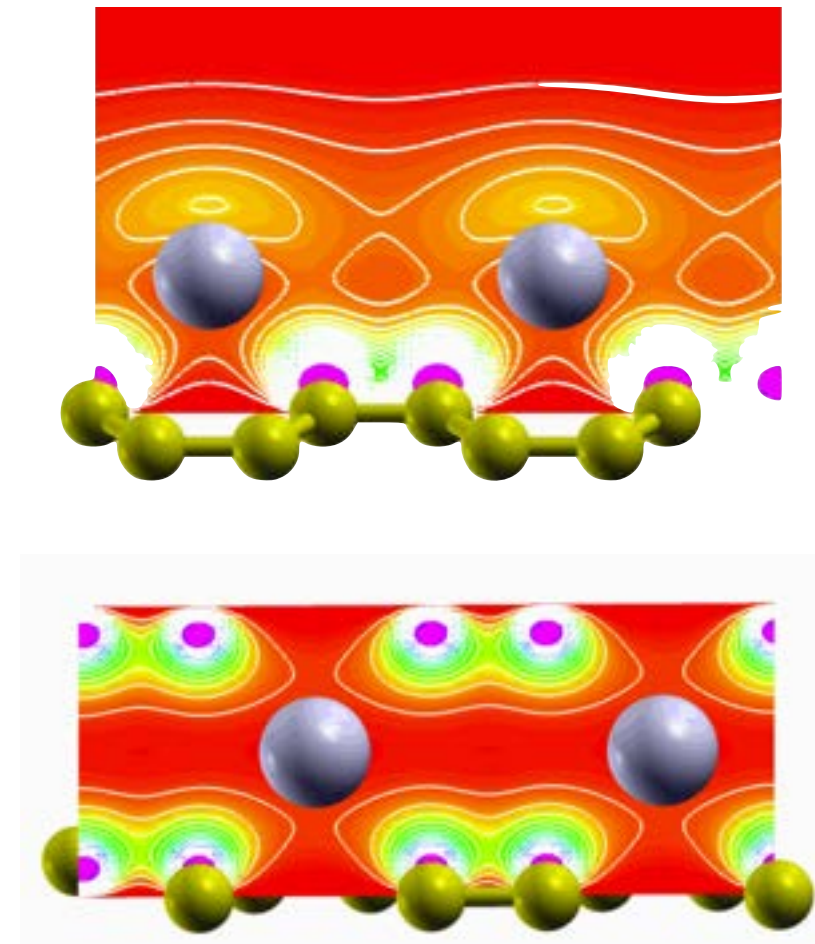
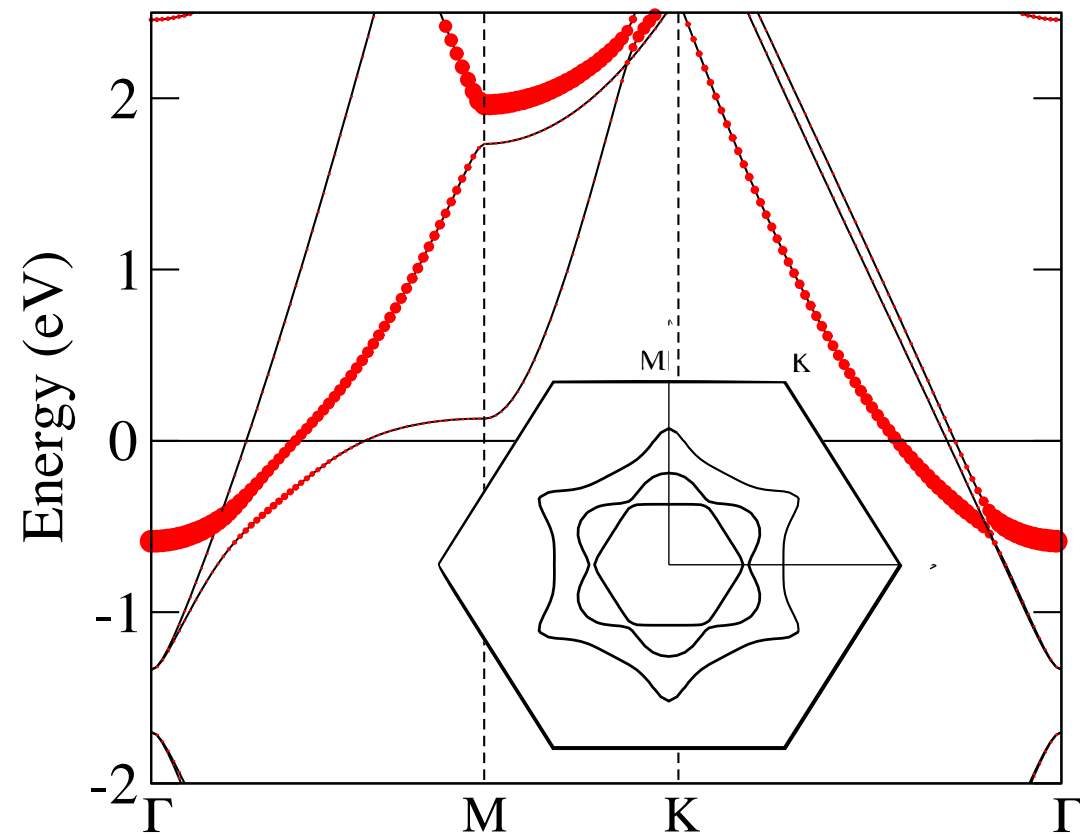
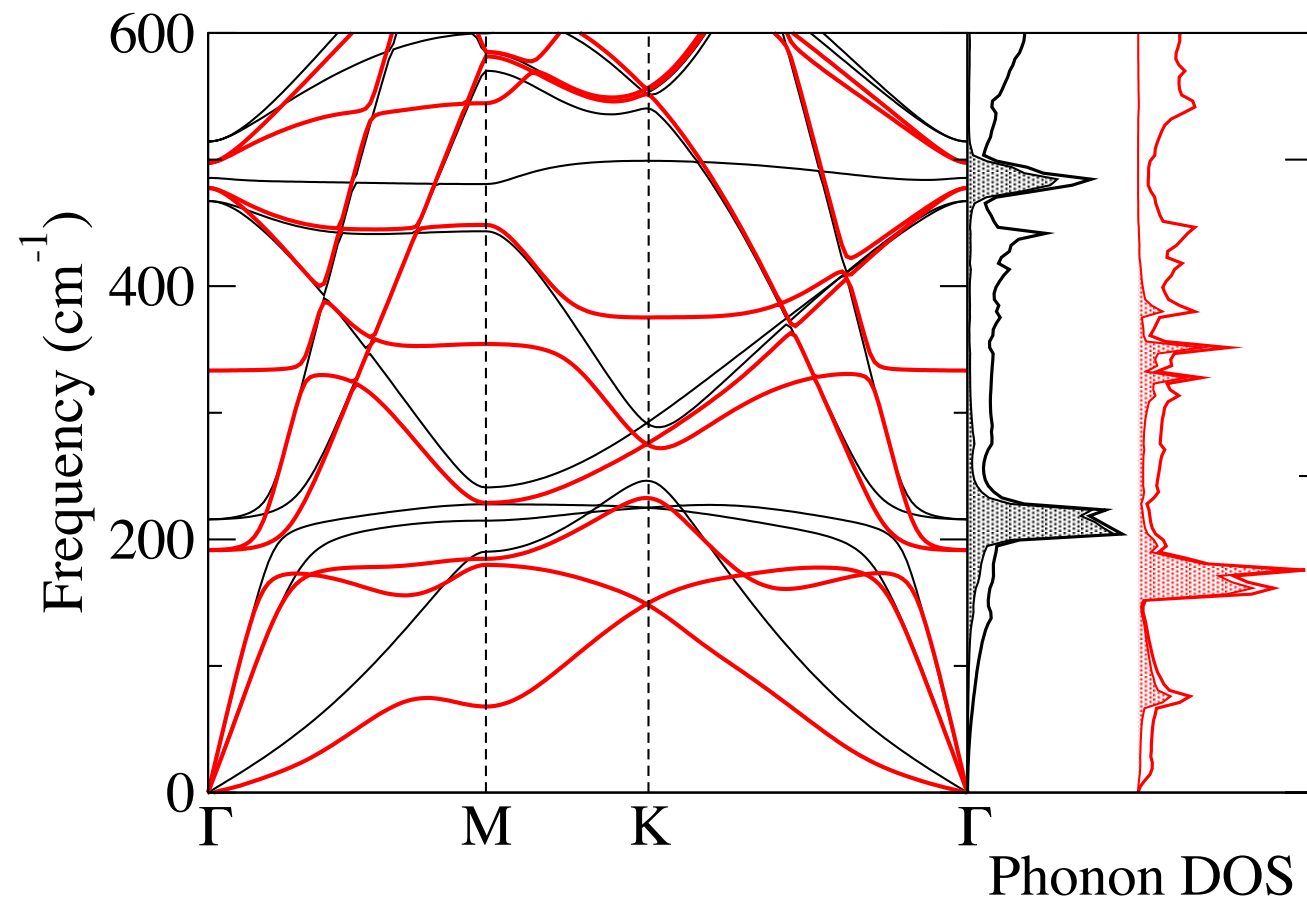
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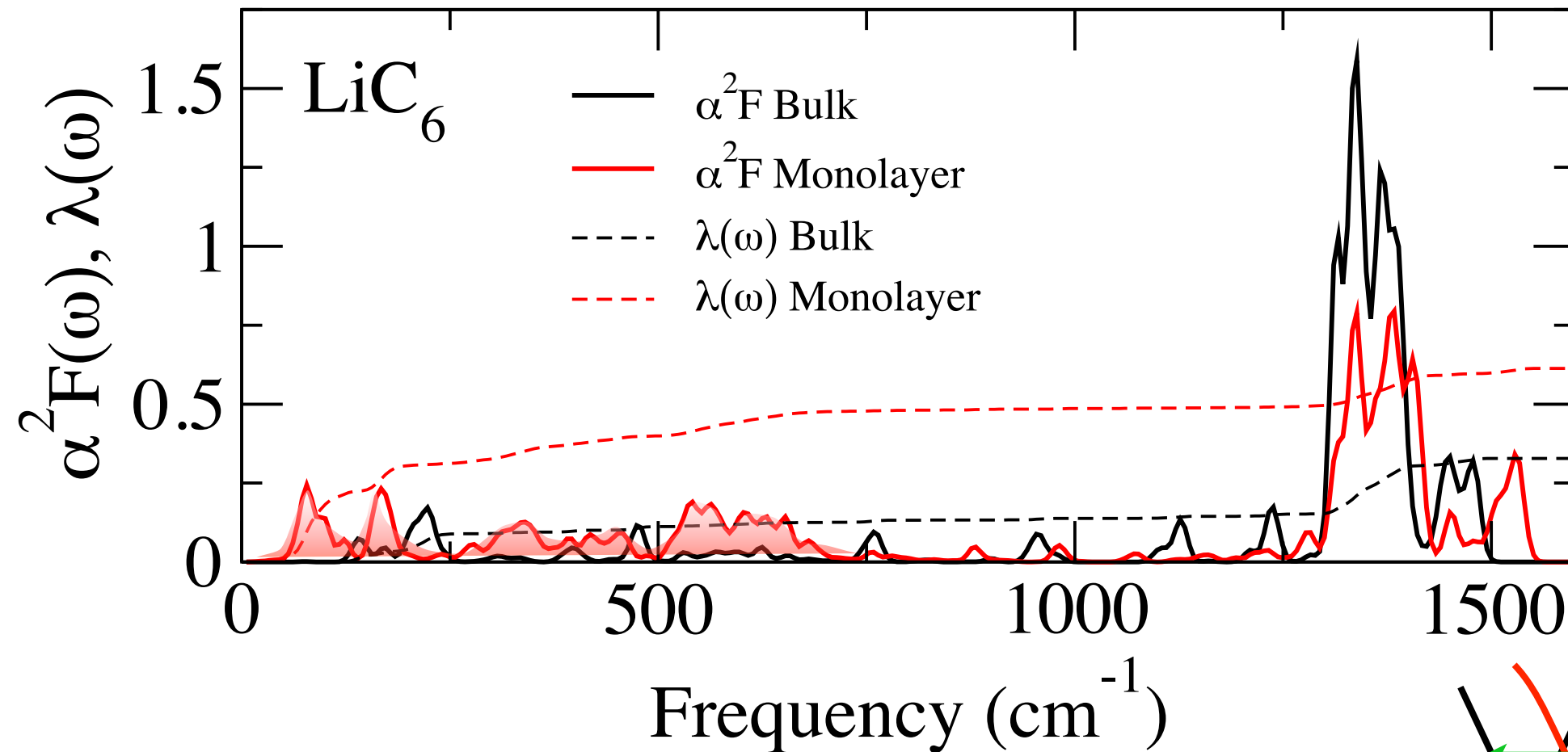
Lithium doped Graphene



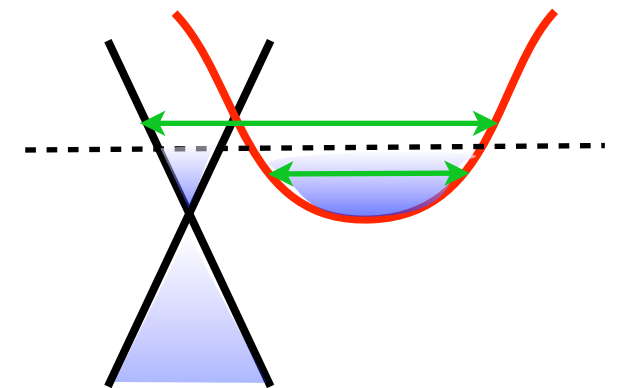
- IL state at the Fermi level
- Softening of Li and C_z modes
- Increase of DOS at E_F

Lithium doped Graphene

Electron-phonon coupling

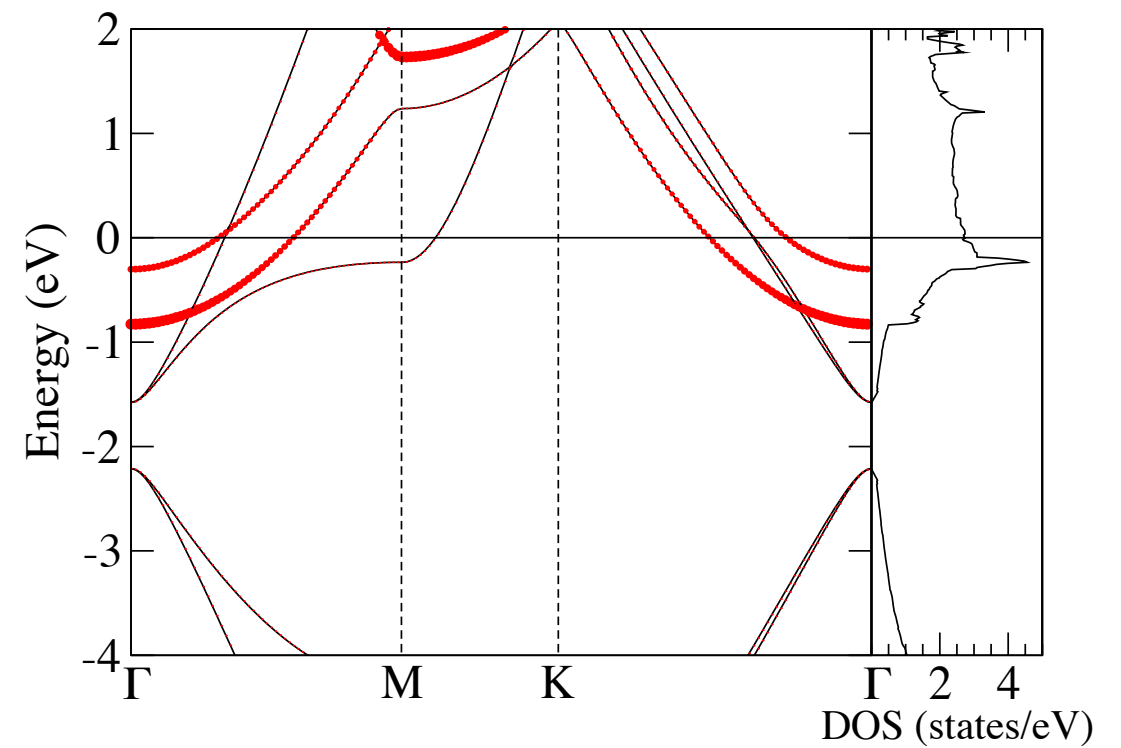
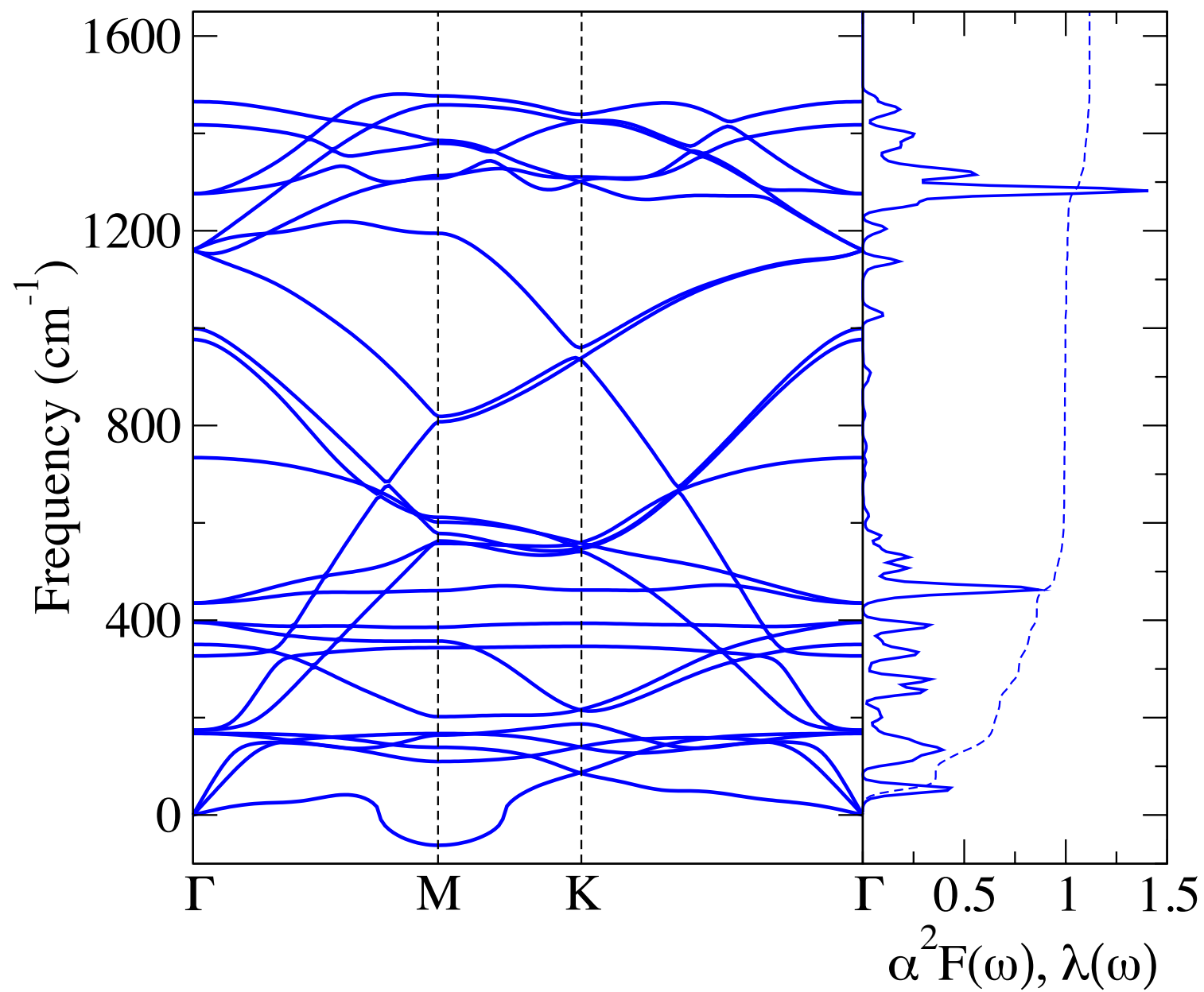
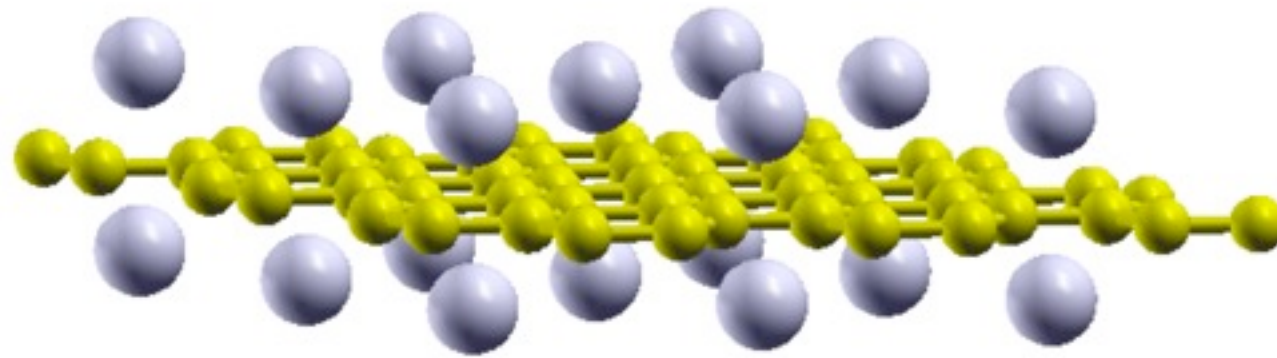


- Bulk LiC₆ is not superconducting (no interlayer state)
- The interlayer state allows the coupling with “dormant” C_z modes
- Increases the DOS at the Fermi level
- Allows an additional intra-band and 2 inter-band scattering channels



- Increases the total electron-phonon coupling to $\lambda = 0.61$ and $T_c = 8.1$ K

Lithium on both sides of Graphene



$\lambda = 1.0$ and $T_c = 18 \text{ K}$

Conclusions

- Rigid doping can not induce electron-phonon driven superconductivity
- Metal adatoms on graphene promotes the interlayer state at the Fermi level
- The coupling depends on the particular adatom, very different from the bulk counterpart
- Lithium on graphene has a sizable electron-phonon coupling
- and can induce superconductivity.

“How to make graphene superconducting”

G. Profeta, M. Calandra and F. Mauri

cond-mat arXiv: xxx.xxxx

Thank you
for your attention

