ab initio calculations in novel superconductors

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CONICET

Outline

- MgB_2 : Why T_c = 39 K?
- Superconductors discovered after MgB_2.
- Results obtained for OsN_2 (*Physical Review B 77, 092504 (2008)*).
- Conclusions

ab initio calculations in colaboration with:

- Sandro Scandolo
  (ICTP, Italy)

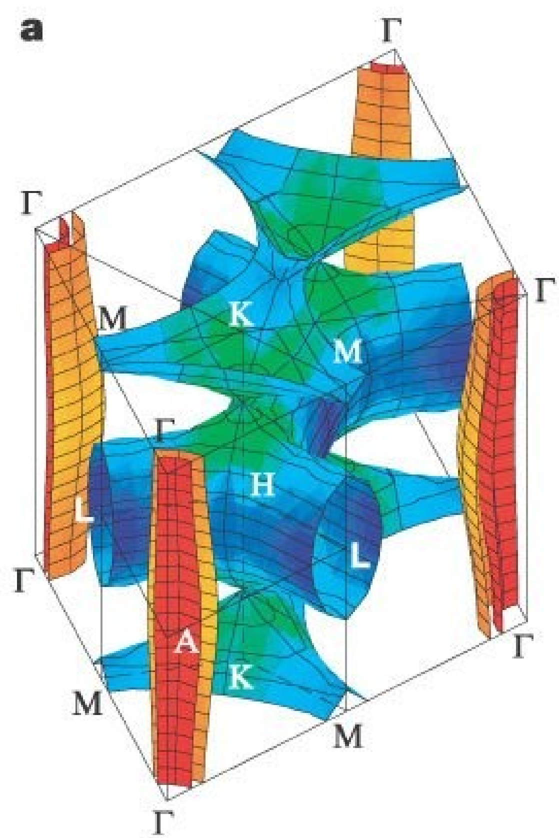
- Gianni Profeta
  (L'Aquila, Italy)
- Javier Montoya
  (Carnegie, USA)

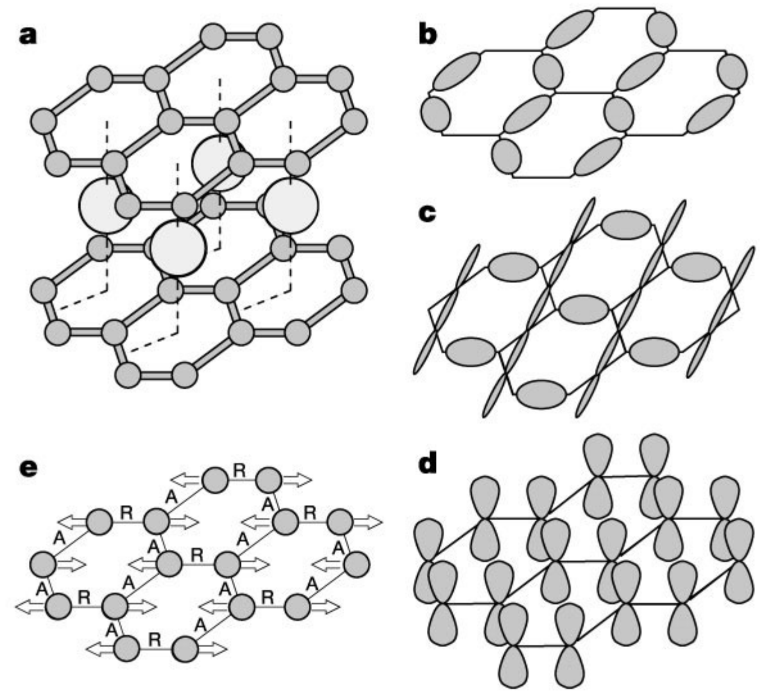
Physical Review B 77, 092504 (2008).

Where is Bariloche?

How is Bariloche?

MgB_2 : Why T_c= 39K?





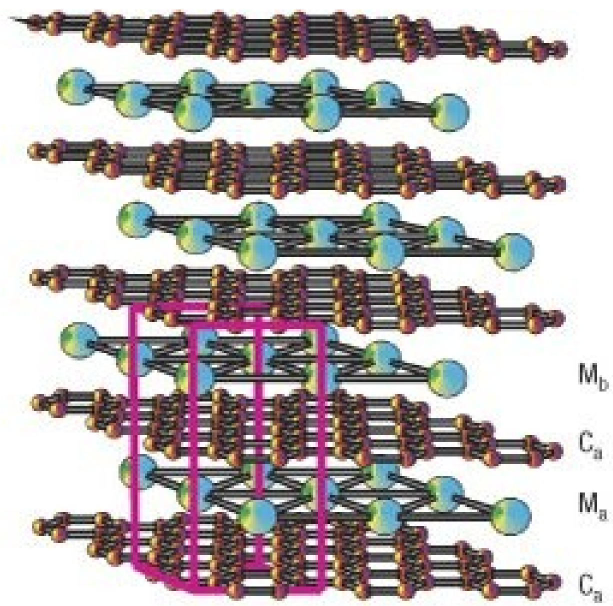
$$T_c = \frac{\langle \omega_{\ln} \rangle}{1.2} \exp\left(- \frac{1.04(1+\lambda)}{\lambda - \mu^*(1+0.62\lambda)} \right)$$

$<\omega_{ln}>$=56meV=650K; λ=1.01

$$\lambda = N(0)\langle I^2 \rangle / M \langle \omega^2 \rangle$$

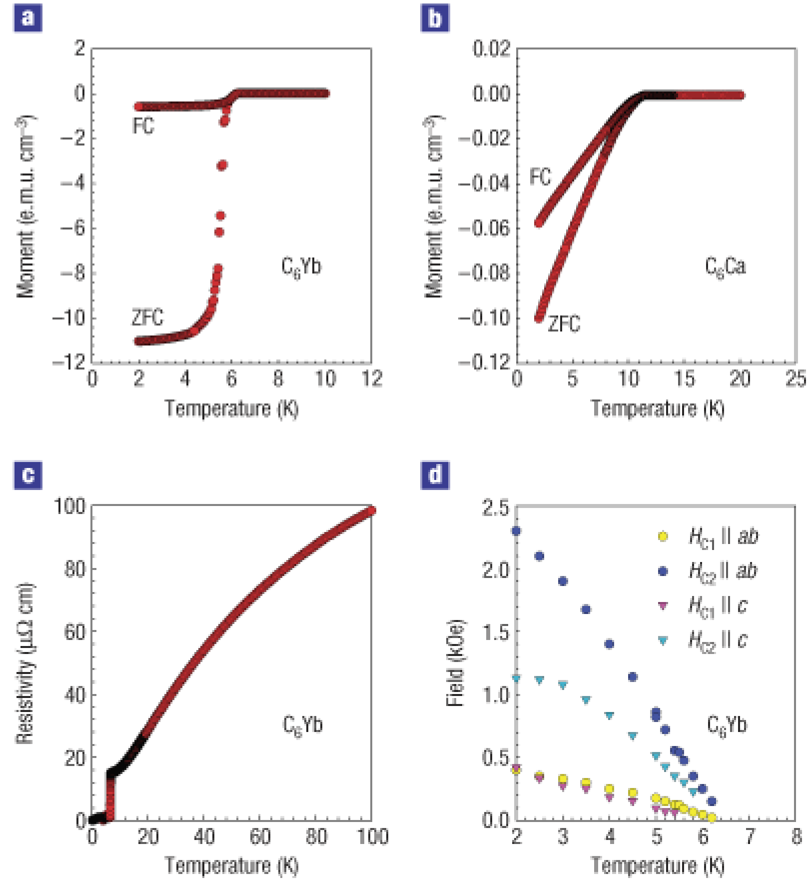
Graphite intercalated compounds

Weller *et al.,* Nature Physics **1**, 39 (2005).



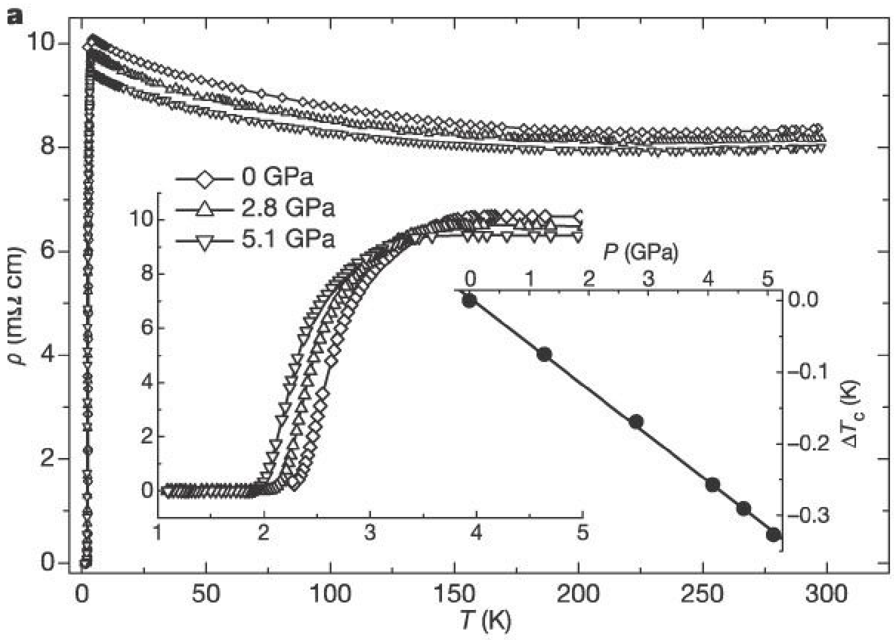
$T_c \approx 6.5$ K

$T_c \approx 11.5$K



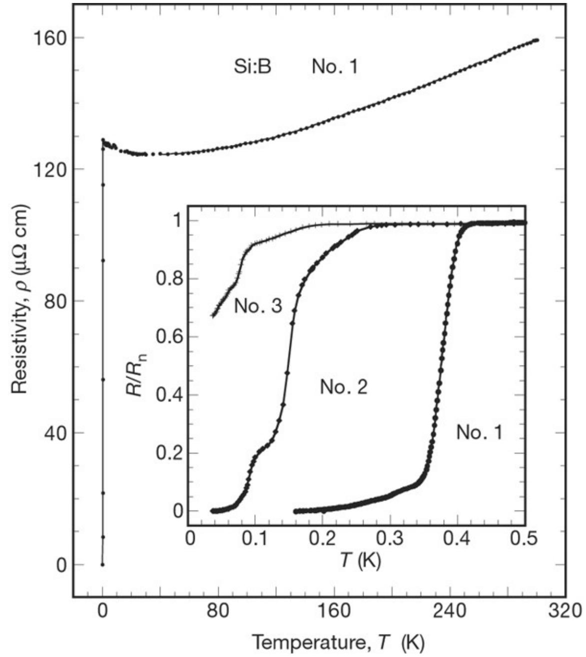
Boron-doped diamond and silicon

Ekimov *et al.,* Nature **428**, 542 (2004).



$T_c \approx 4K$

Bustarret *et al.,* Nature **444**, 465 (2006).



$T_c \approx 0.35K$

Eliashberg Theory of SC

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

$$g^{\nu}_{\mathbf{k}n,\mathbf{k}+\mathbf{q}m} = \langle \mathbf{k}n | \delta V / \delta u_{\mathbf{q}\nu} | \mathbf{k}+\mathbf{q}m \rangle / \sqrt{2\omega_{\mathbf{q}\nu}}$$

$$\lambda_{\mathbf{q}\nu} = \frac{4}{\omega_{\mathbf{q}\nu} N(E_F) N_k} \sum_{\mathbf{k},n,m} |g^{\nu}_{\mathbf{k}n,\mathbf{k}+\mathbf{q}m}|^2 \delta(\epsilon_{\mathbf{k}n}) \delta(\epsilon_{\mathbf{k}+\mathbf{q}m})$$

$$\lambda = \sum_{\mathbf{q}\nu} \lambda_{\mathbf{q}\nu} / N_q$$

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

$$\lambda(\omega) = 2 \int_0^{\omega} d\omega' \alpha^2 F(\omega') / \omega'$$

SCDFT

Oliveira, Gross, and Khon, PRL (1998).
PRB 72, 024545 (2005); PRB 72, 024546 (2005)
PRL 96, 047003 (2006); PRL 96, 047003 (2006); etc

$$\Delta_{n\mathbf{k}} = -Z_{n\mathbf{k}}\Delta_{n\mathbf{k}} - \frac{1}{2}\sum_{n'\mathbf{k}'}\mathcal{K}_{n\mathbf{k},n'\mathbf{k}'}\frac{\tanh(\frac{\beta}{2}E_{n'\mathbf{k}'})}{E_{n'\mathbf{k}'}}\Delta_{n'\mathbf{k}'}$$

$$\mathcal{K} = \mathcal{K}^{e\text{-ph}} + \mathcal{K}^{e\text{-}e}$$

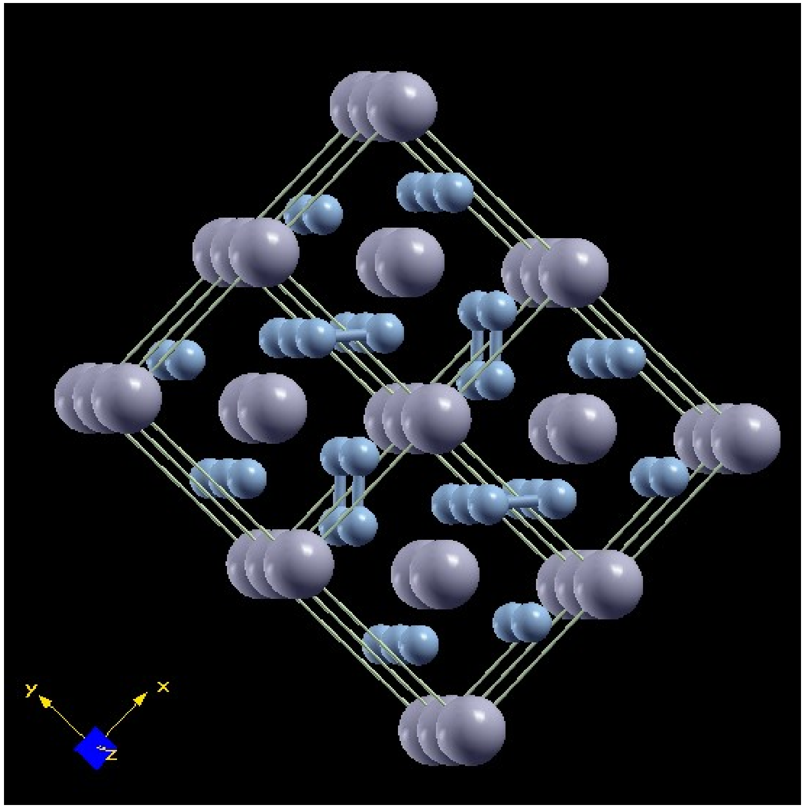
$$E_{n\mathbf{k}} = \sqrt{(\varepsilon_{n\mathbf{k}} - \mu)^2 + |\Delta_{n\mathbf{k}}|^2}$$

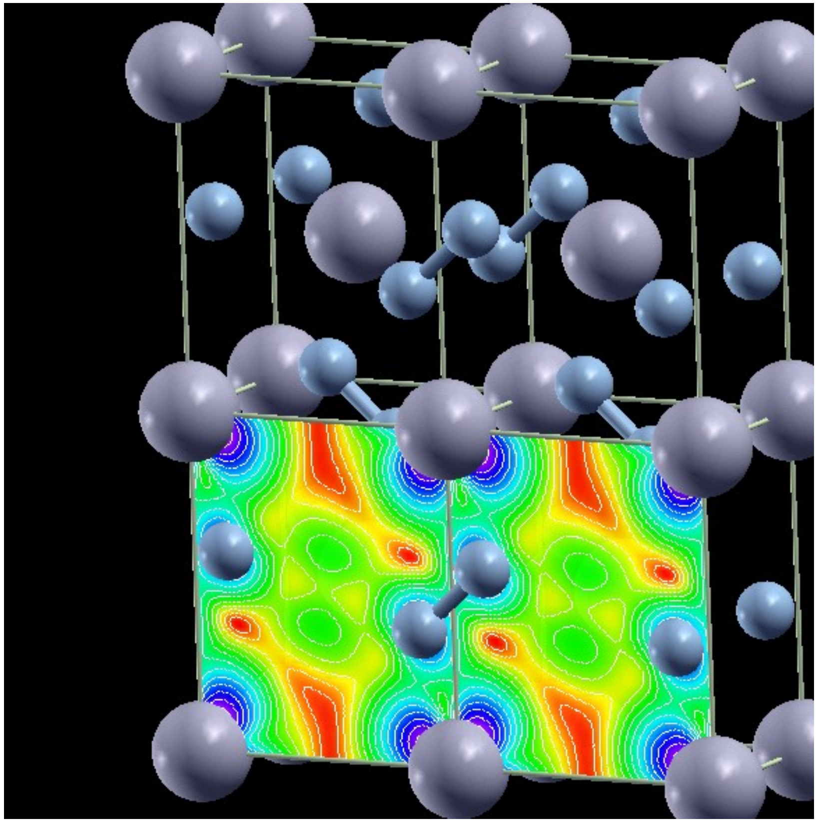
$$\Delta(\xi) = -\mathcal{Z}(\xi)\Delta(\xi) - \frac{1}{2}\int_{-\mu}^{\infty} d\xi' N(\xi')\mathcal{K}(\xi,\xi')\frac{\tanh[(\beta/2)E']}{E'}\Delta(\xi')$$

$$\mathcal{K}^{\text{TF-FE}}(\xi,\xi') = \frac{\pi}{kk'}\ln\left[\frac{(k+k')^2 + k_{\text{TF}}^2}{(k-k')^2 + k_{\text{TF}}^2}\right]$$

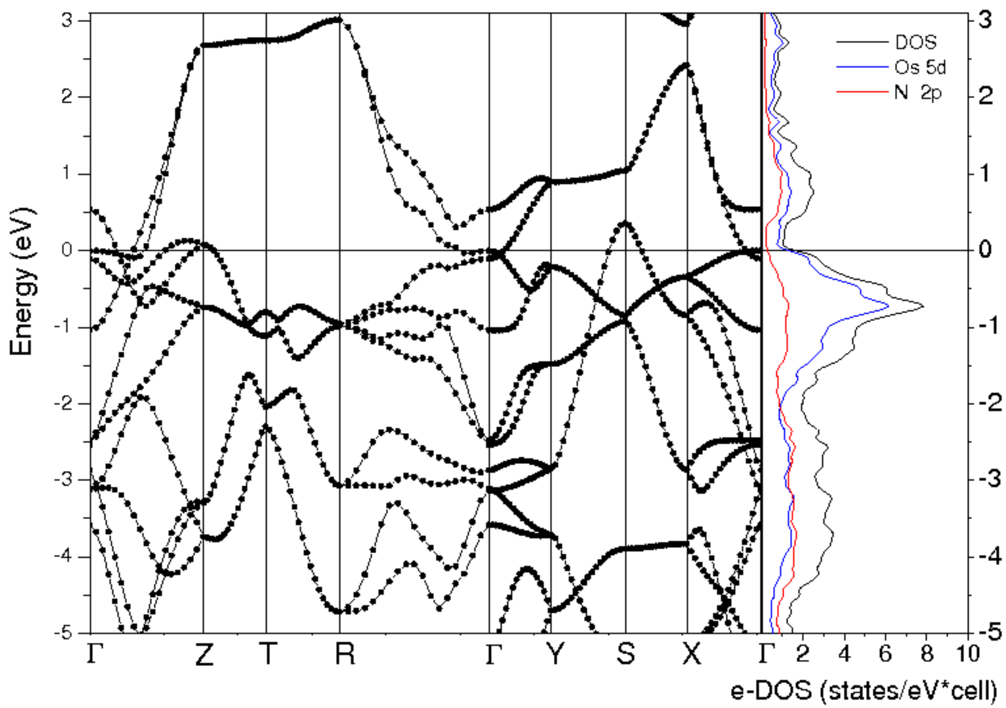
OsN_2

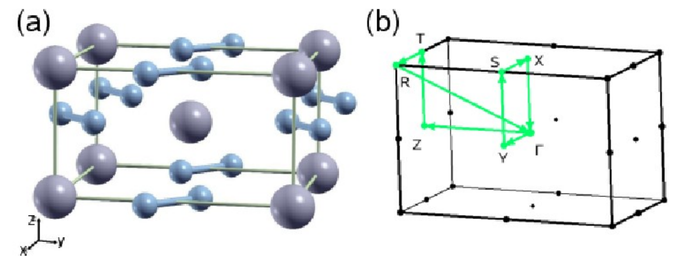
Appl. Phys. Lett. **90**, 011909 (2007).
Physical Review B 77, 092504 (2008).

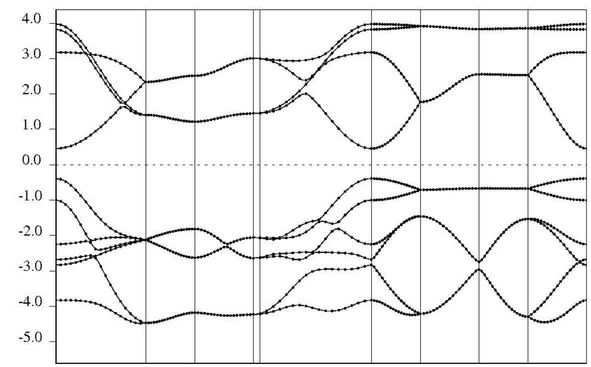




Electronic properties of OsN_2

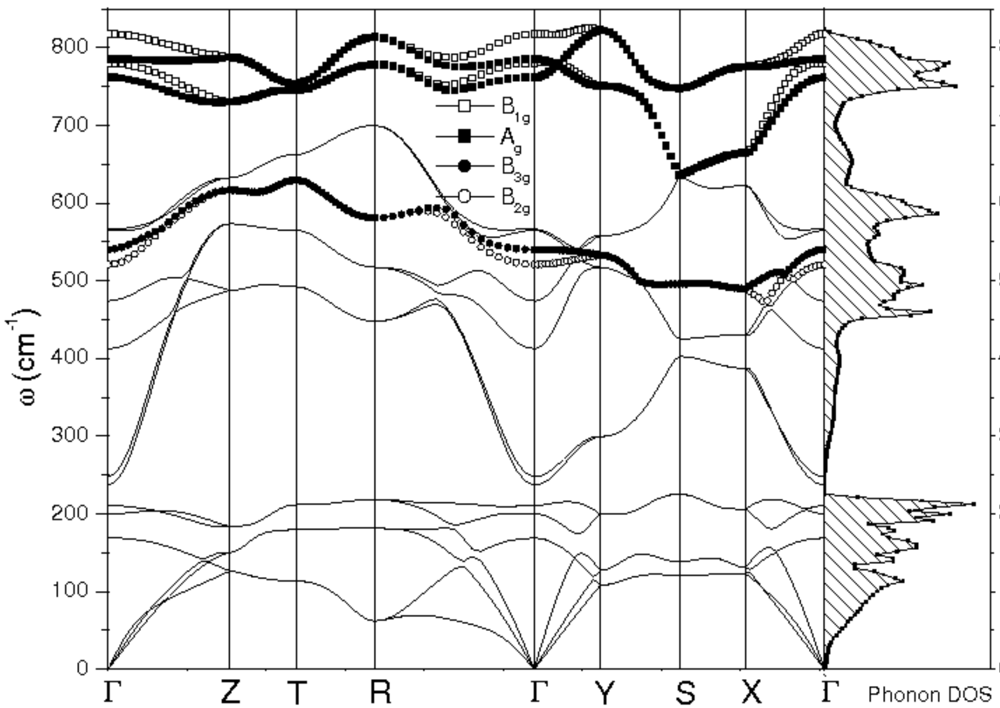


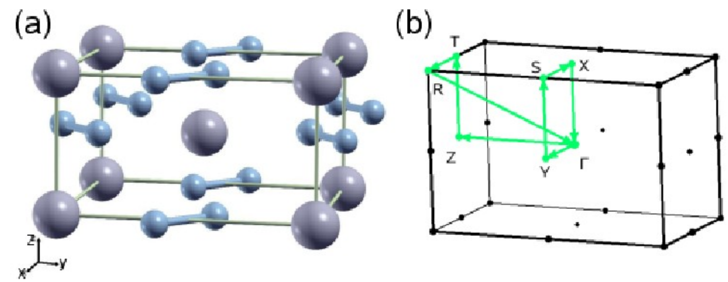




- the N 2p orbitals contribute with about 20% of the total DOS(E_f)
- 92% of the nitrogen contribution at E_f is due to N $p_{x,y}$ states

Phonons dispersions of OsN_2





B_{2g} y B_{3g} 1 mode

A_g y B_{1g} 2 modes

B_{2g} y A_g in phase

B_{3g} y B_{1g} counterphase

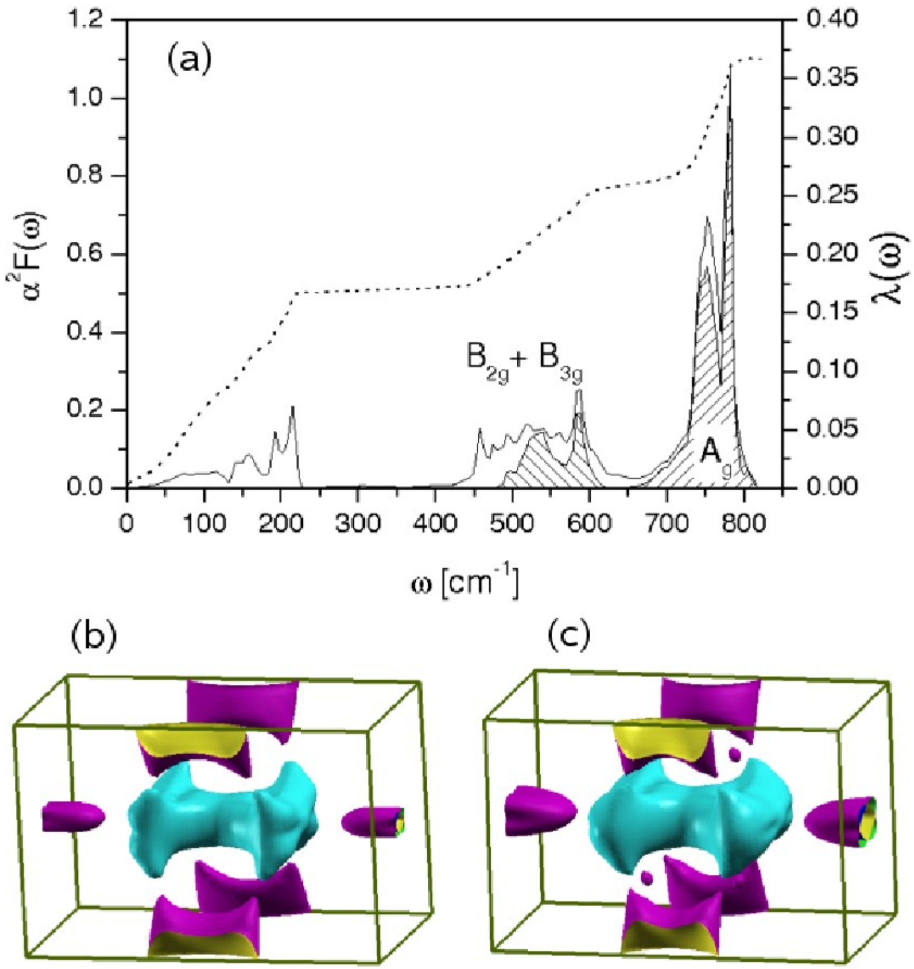
N-N $\omega \approx 2300\ cm^{-1}$

$$C_{\alpha i,\beta j}(\mathbf{R}-\mathbf{R}') = \left.\frac{\partial^2 E}{\partial u_{\alpha i}(\mathbf{R})\partial u_{\beta j}(\mathbf{R}')}\right|_{\text{equil}}$$

$$\omega^2(\mathbf{q})u_{\alpha i}(\mathbf{q}) = \sum_{\beta j} u_{\beta j}(\mathbf{q})\tilde{D}_{\alpha i,\beta j}(\mathbf{q})$$

$$\tilde{D}_{\alpha i,\beta j}(\mathbf{q}) = \frac{1}{\sqrt{M_i M_j}}\sum_{\mathbf{R}} C_{\alpha i,\beta j}(\mathbf{R})e^{-i\mathbf{q}\cdot\mathbf{R}}$$

Electron-phonon interaction



$$\lambda(\omega) = 2\int_0^{\omega} d\omega' \alpha^2 F(\omega')/\omega'$$

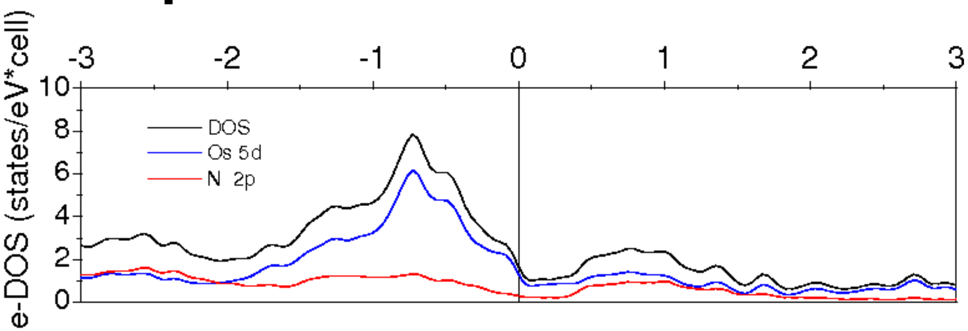
$$T_c = \frac{\langle \omega_{\ln} \rangle}{1.2} \exp\left(-\frac{1.04(1+\lambda)}{\lambda - \mu^*(1+0.62\lambda)}\right)$$

$<\omega_{ln}>=280K$; $\lambda = 0.37$

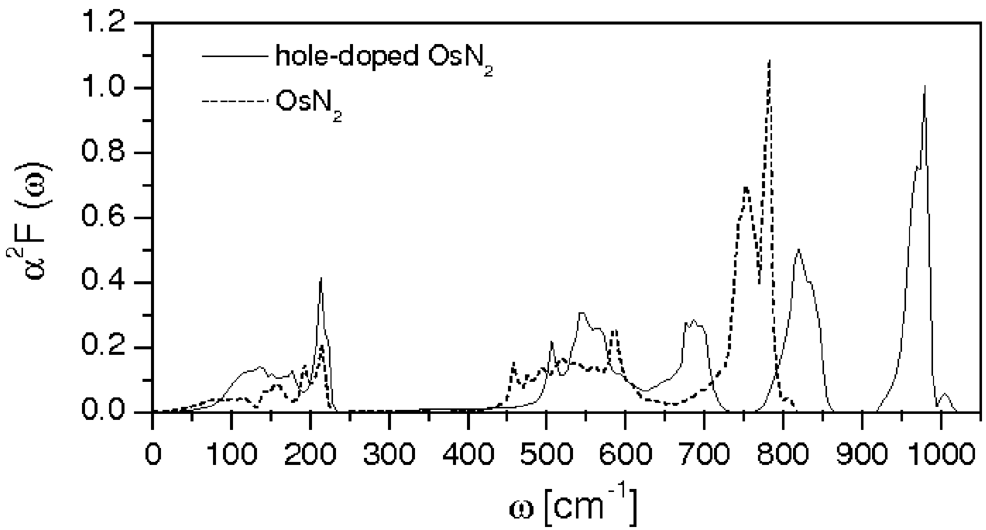
$0.3<T_c<1.2$ for $0.13> \mu^* >0.08$

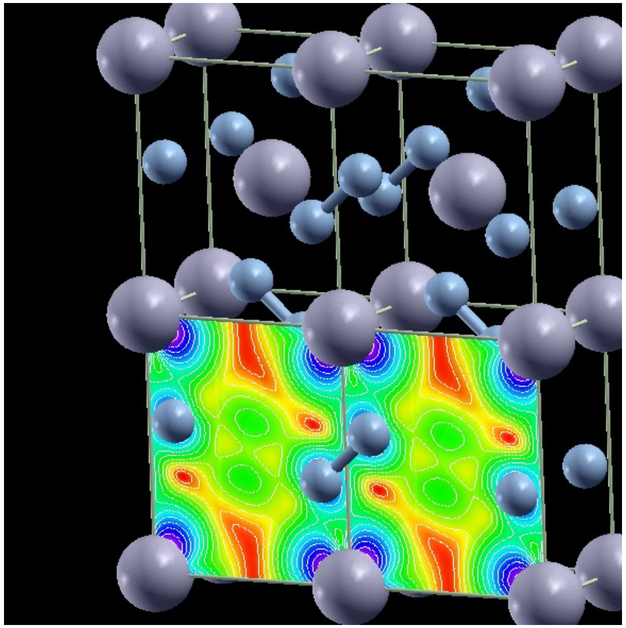
$T_c \approx 1K$ at $\mu^* = 0.1$

Hole-doped OsN_2



$$\lambda = N(0)\langle I^2\rangle / M\langle\omega^2\rangle$$



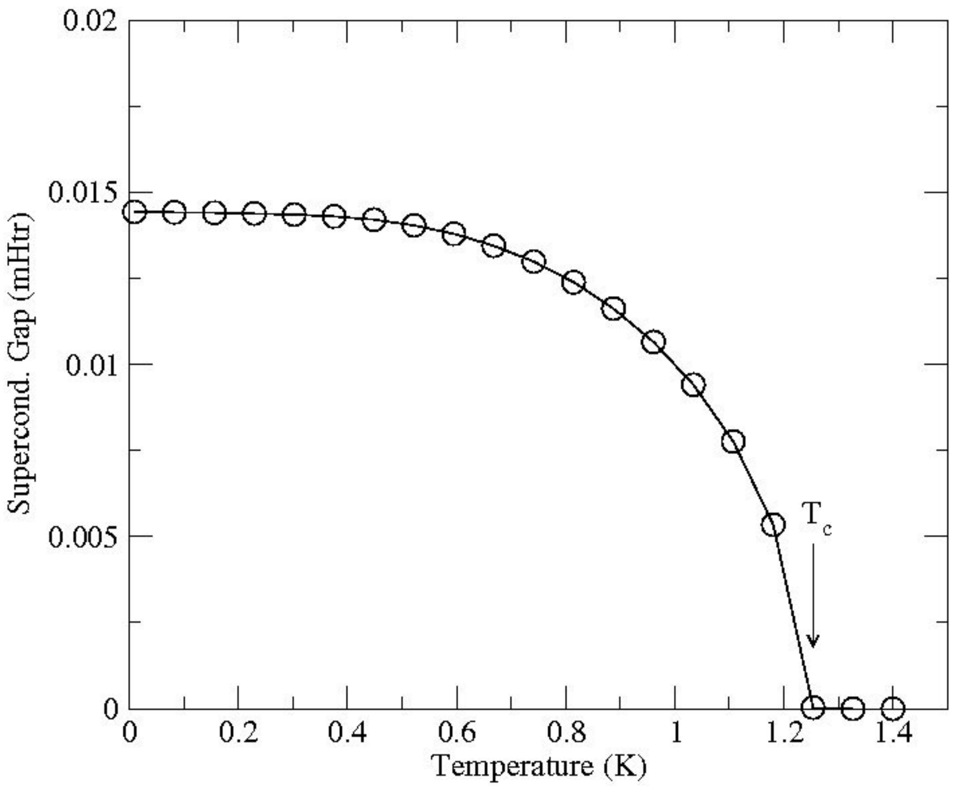


eDOS increases 2.4 times

$\langle\omega_{ln}\rangle$ = 310K ; λ = 0.49

$T_c \approx$ 4K for μ^*=0.1

Results using the SCDFT



$$\Delta(\xi) = -\mathcal{Z}(\xi)\Delta(\xi) - \frac{1}{2}\int_{-\mu}^{\infty} d\xi' N(\xi')\mathcal{K}(\xi,\xi')\frac{\tanh[(\beta/2)E']}{E'}\Delta(\xi')$$

$$\mathcal{K}^{\text{TF-FE}}(\xi,\xi') = \frac{\pi}{kk'}\ln\left[\frac{(k+k')^2 + k_{\text{TF}}^2}{(k-k')^2 + k_{\text{TF}}^2}\right]$$

CONCLUSIONS

- We predict that OsN_2 is a superconductor.
- Its superconducting properties are connected with a strong coupling between the stretching modes of the covalently bonded N_2 units with the electronic states at the Fermi level.
- Our calculations predict an enhancement of the superconducting temperature by doping OsN_2 with holes.