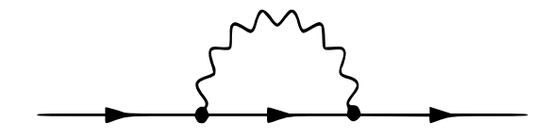
Zero-point phonon renormalization of the band gap of materials

Michel Côté

Université de Montréal

Collaborators



Gabriel Antonius

now at Berkeley

Samuel Poncé

now at Oxford

Paul Boulanger

Xavier Gonze

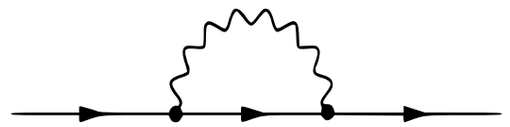
Université de Montréal

UCL Université catholique de Louvain

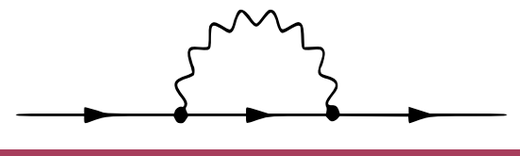
UNIVERSITAS CATHOLICA LOVANIENSIS SEDES SAPIENTIAE 1425

NÉEL institut

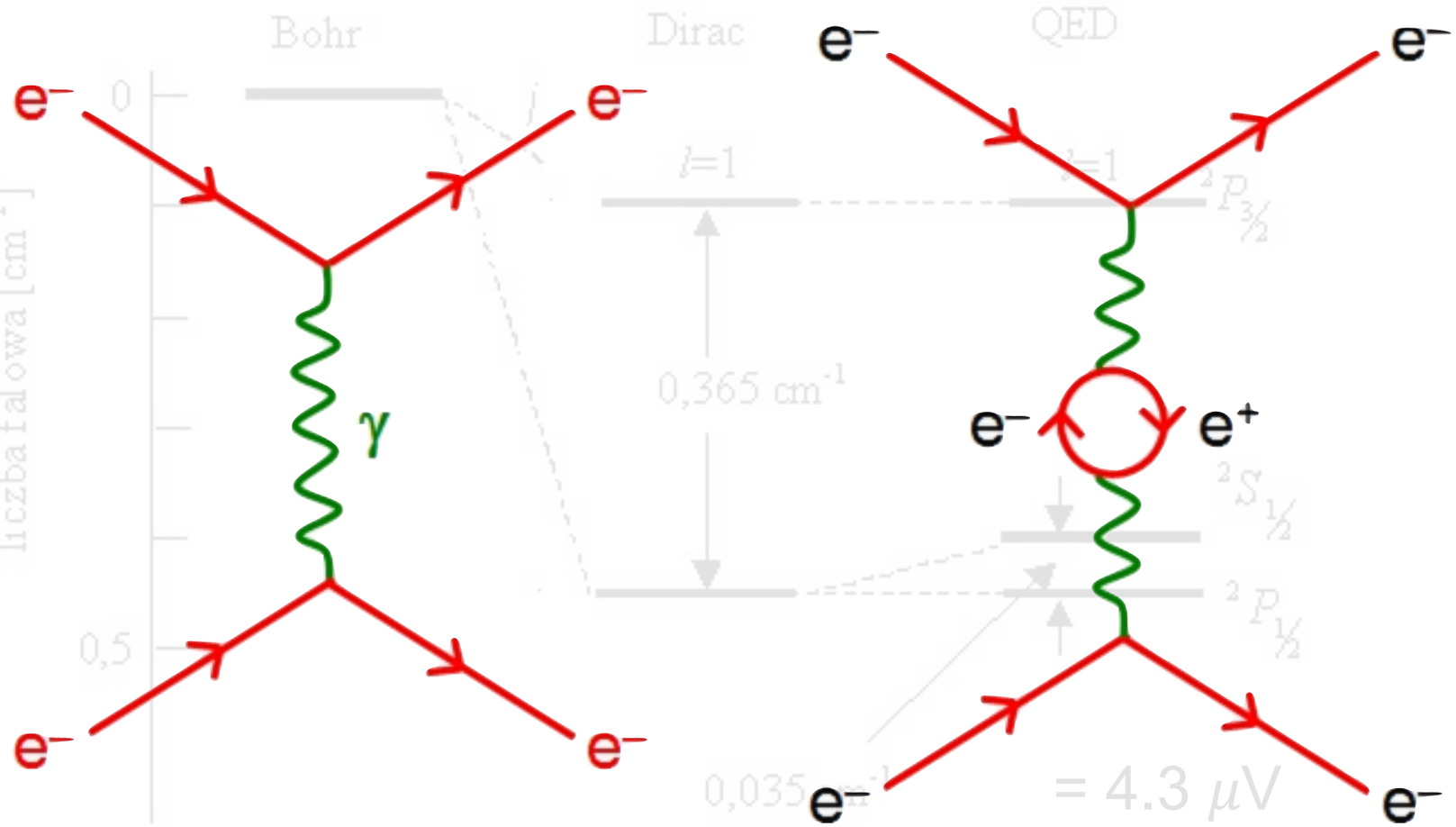
Outline



- Introduction/Motivations
- Theory: Allen-Heine-Cardona
- Calculations for diamond
  - at the density-functional theory level
  - at the GW method level
  - including anharmonic effects
  - including dynamical effects
- Conclusion



Quantum Electrodynamics (QED)

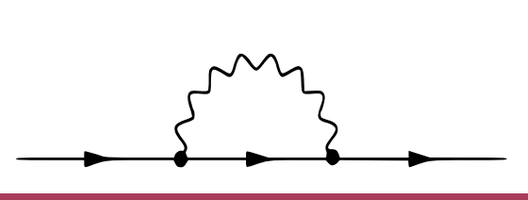


[H. Haken, H.C.Wolf, Atomic Physics, 1996]

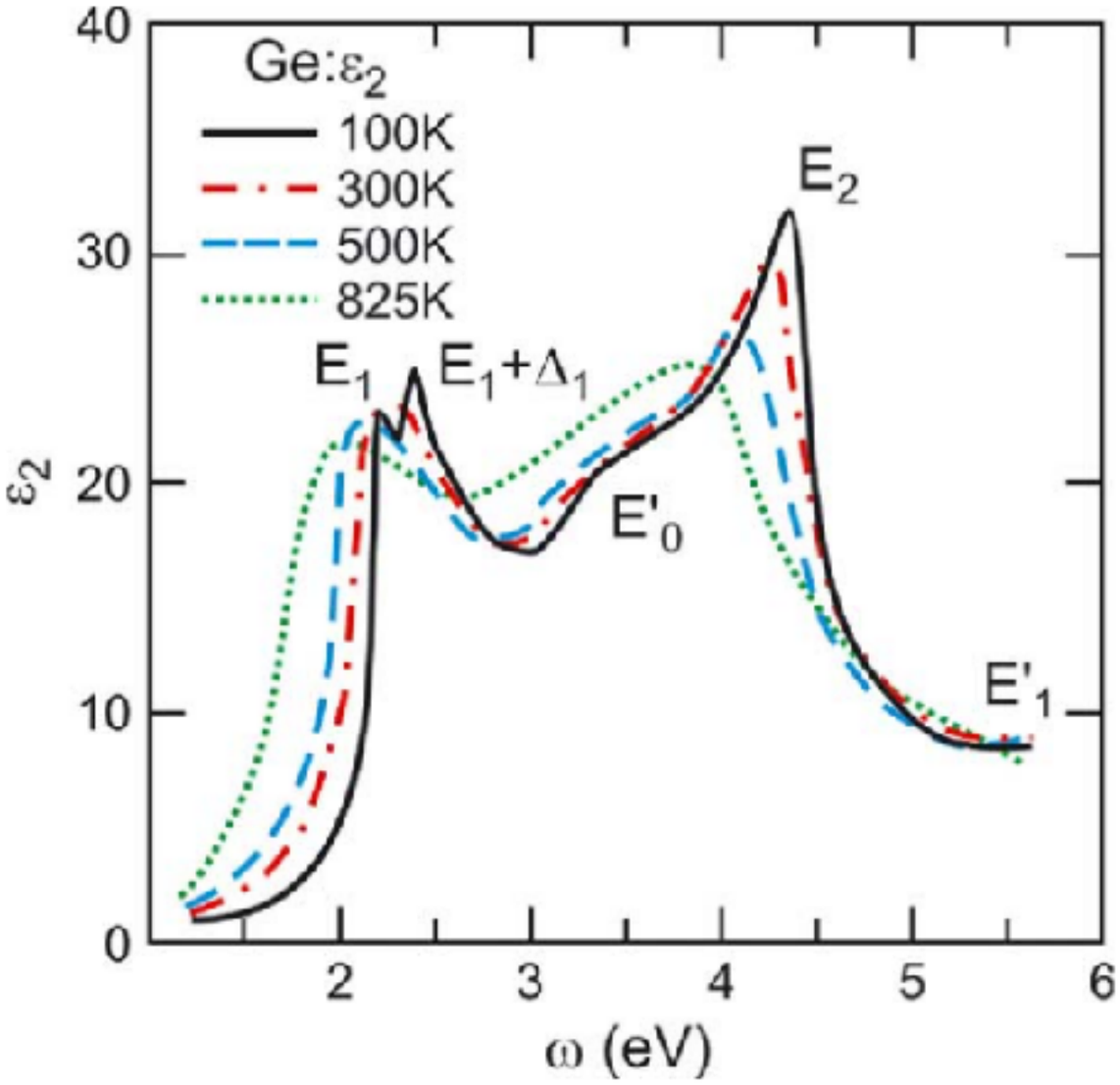
Vacuum is never empty.

Condensed matter: photons → phonons

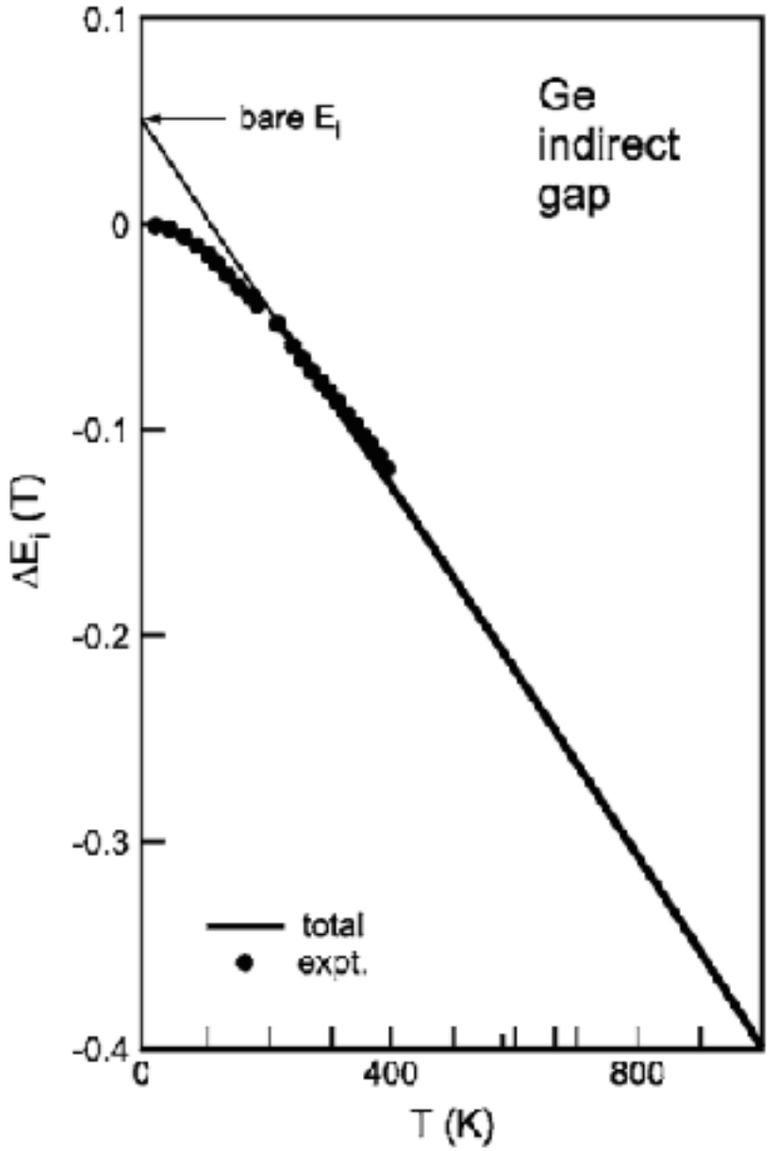
Eg vs T



Germanium

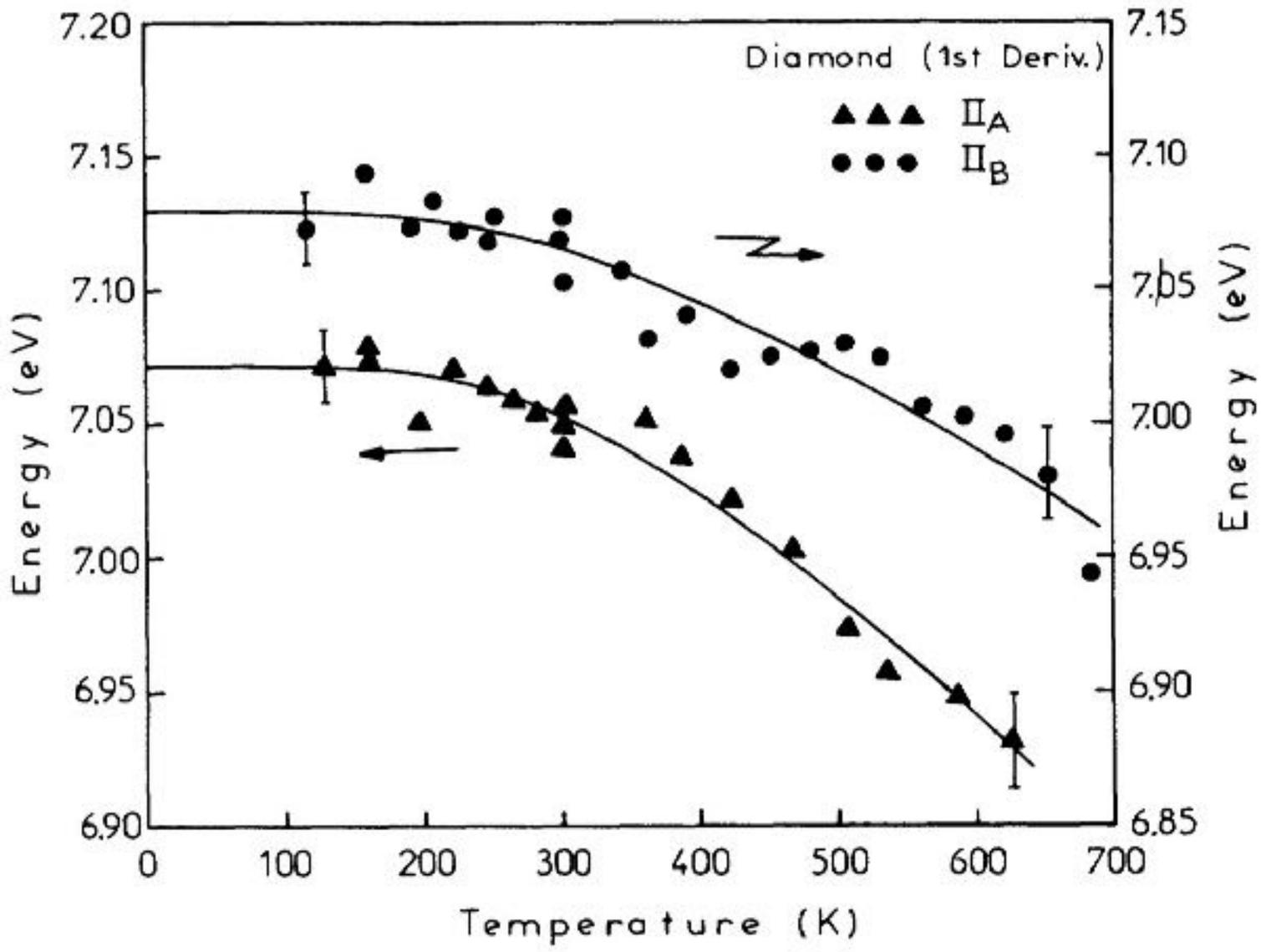


L. Viña, S. Logothetidis and M. Cardona, Phys. Rev. B **30**, 1979 (1984)



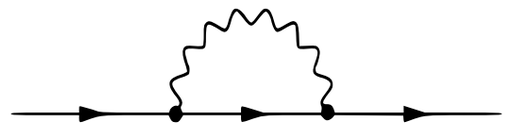
Cardona and Thewalt, *Rev. Mod. Phys.*,77, 1173 (2005)

Eg vs T: Diamond



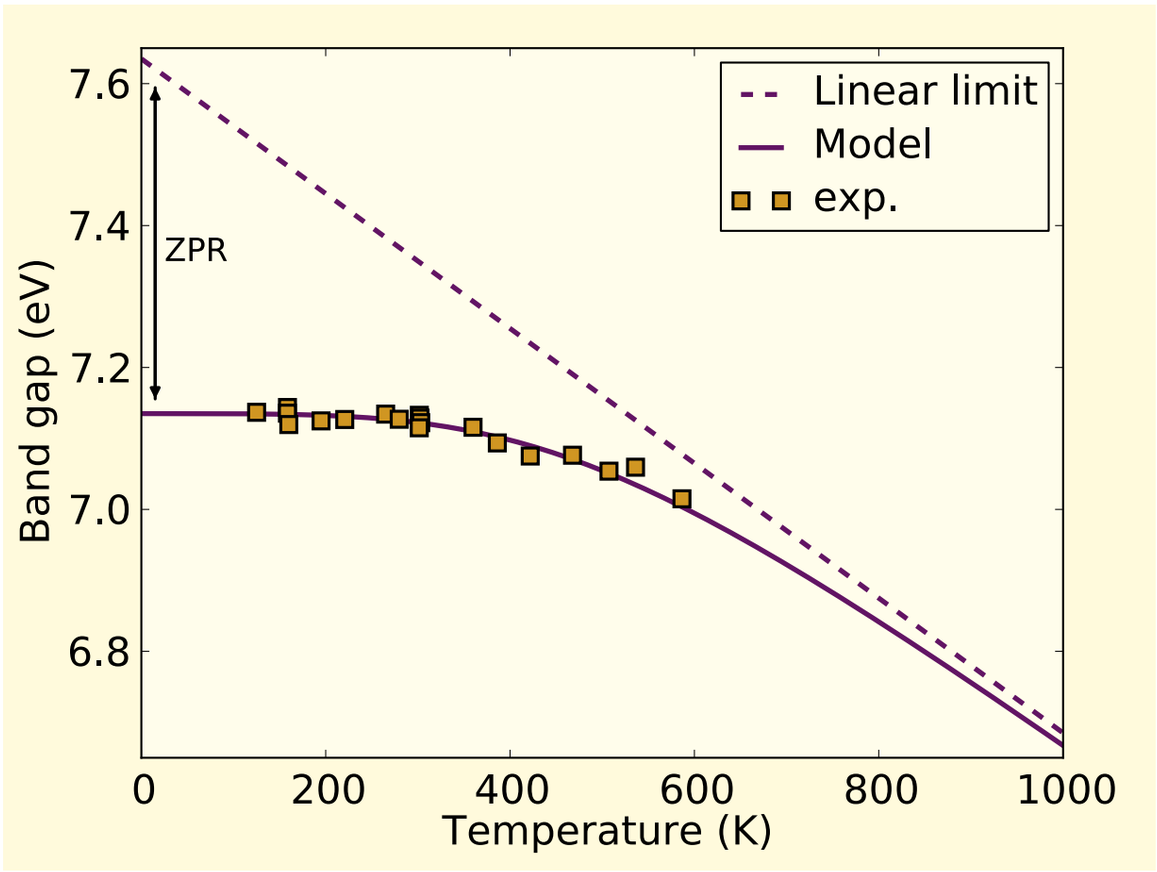
Logothetidis et al., *Phys Rev B,* 46, 4483 (1992)

Eg vs T



Varshni formula:

$$E(T) = E_o - a\frac{T^2}{T+\beta}$$

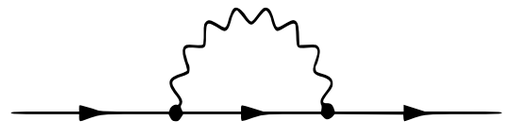


ZPR: Zero Point Renormalization

	ZPR (meV)
Silicon	64
Gemanium	47
GaAs	54
Diamond (ind)	370
Diamond (direct)	600-700

ref: Cardona and Thewalt, *Rev. Mod. Phys.*,77, 1173 (2005)
Logothetidis et al., *Phys Rev B,* 46, 4483 (1992).

High precision *ab initio* calculations



PRL **99,** 246403 (2007) PHYSICAL REVIEW LETTERS week ending 14 DECEMBER 2007

Accurate Quasiparticle Spectra from Self-Consistent *GW* Calculations with Vertex Corrections

M. Shishkin, M. Marsman, and G. Kresse

Faculty of Physics, Universität Wien and Center for Computational Materials Science, Sensengasse 8/12, A-1090 Wien, Austria

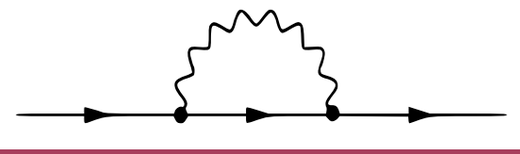
(Received 21 June 2007; published 12 December 2007)

	Δ (eV)			
	scGW RPA	scGW e-h	GW_0^{DFT} RPA	EXP
Ge	0.95	0.81	0.75	0.74
Si	1.41	1.24	1.28 (1.20)	1.17
GaAs	1.85	1.62	1.55 (1.42)	1.52
SiC	2.88	2.53	2.62 (2.45)	2.40
CdS	2.87	2.39	2.37 (2.28)	2.42
AlP	2.90	2.57	2.57 (2.59)	2.45
GaN	3.82	3.27	3.30 (3.00)	3.20
ZnO	3.8	3.2	3.0 (2.5)	3.44
ZnS	4.15	3.60	3.59 (3.50)	3.91
C	6.18	5.79	5.88 (5.68)	5.48
BN	7.14	6.59	6.66 (6.35)	≈6.25
MgO	9.16	8.12	8.25 (7.64)	7.83
LiF	15.9	14.3	14.8 (14.0)	14.20
Ar	14.9	13.9	14.0 (13.9)	14.20
Ne	22.1	21.4	21.1 (20.5)	21.70

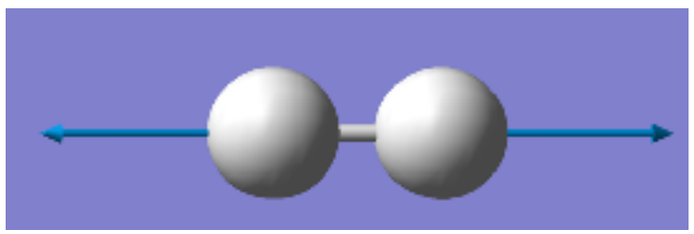
errors ~ 10 meV

errors ~ 500 meV

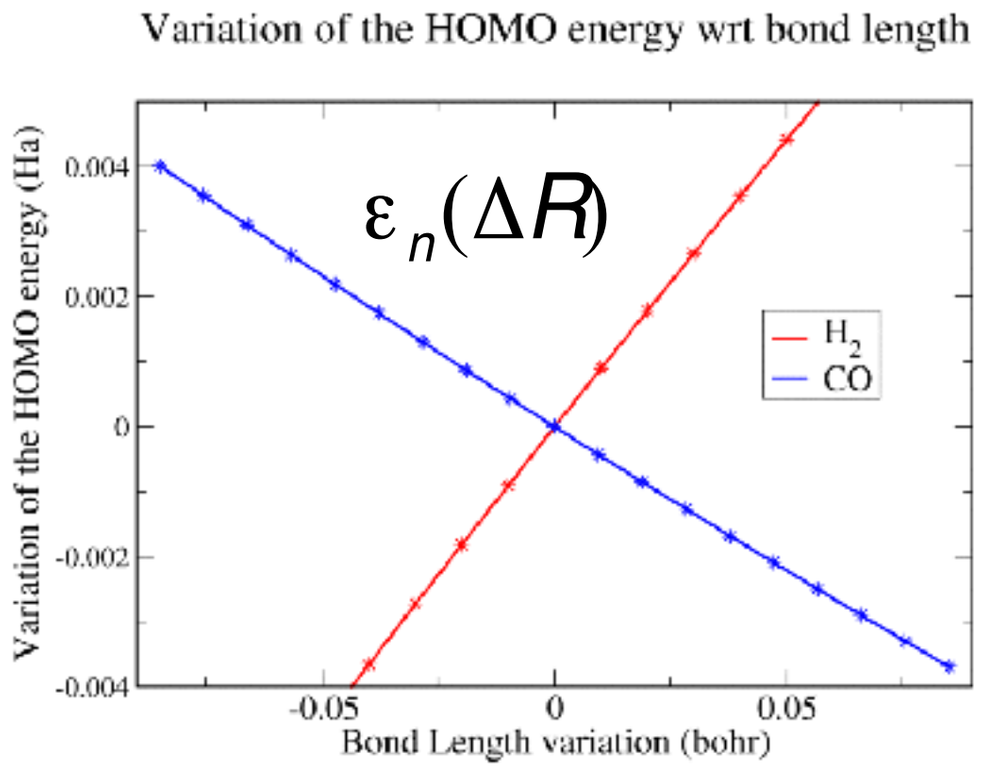
The phonon population contribution: Diatomic molecules



Simple :
discrete levels, simple molecular orbitals
only one relevant vibration mode.



(6 modes decouple as 3 translations, 2 rotations + the stretch.)



One possible solution…

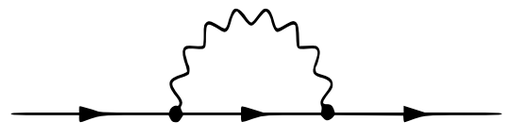
Time-average of eigenenergies from Molecular Dynamics trajectories, at average T

$$\varepsilon_n(T) = \lim_{\tau\to\infty} \frac{1}{\tau} \int_0^{\tau} \varepsilon_n(\Delta R(t))\, dt$$

Pros : well-defined procedure ; compatible with current implementations and computing capabilities; from DFT or GW ; anharmonicities

Cons : if classical dynamics => no zero-point motion ;
adiabatic (vibrations, but no exchange of energy !) ;
hard for solids (supercell), also supercell mix eigenstates

The phonon population contribution: Diatomic molecules



Thermal average with quantum vibrational states in the harmonic approximation, and expansion of $\varepsilon_n(\Delta R)$ to second order (quadratic approximation)

$$E_{ph}(n_{vib}) = \hbar\omega(n_{vib} + \frac{1}{2})$$

$$n_{vib}(T) = \frac{1}{e^{-\frac{\hbar\omega}{k_B T}} - 1}$$

T-dependent phonon occupation number (Bose-Einstein)

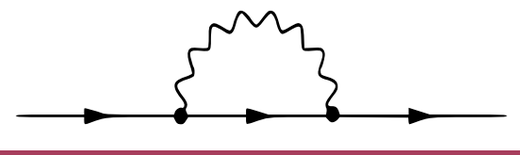
$$\varepsilon_n = \varepsilon_n^0 + \cancel{\frac{\partial \varepsilon_n}{\partial R}\Delta R} + \frac{1}{2}\frac{\partial^2 \varepsilon_n}{\partial R^2}\Delta R^2$$

$$\delta\varepsilon_n(T) = \frac{\partial \varepsilon_n}{\partial n_{vib}}\left(n_{vib}(T) + \frac{1}{2}\right)$$

Pros : zero-point motion ; from DFT or GW ;
tractable … for molecules … ; physical picture

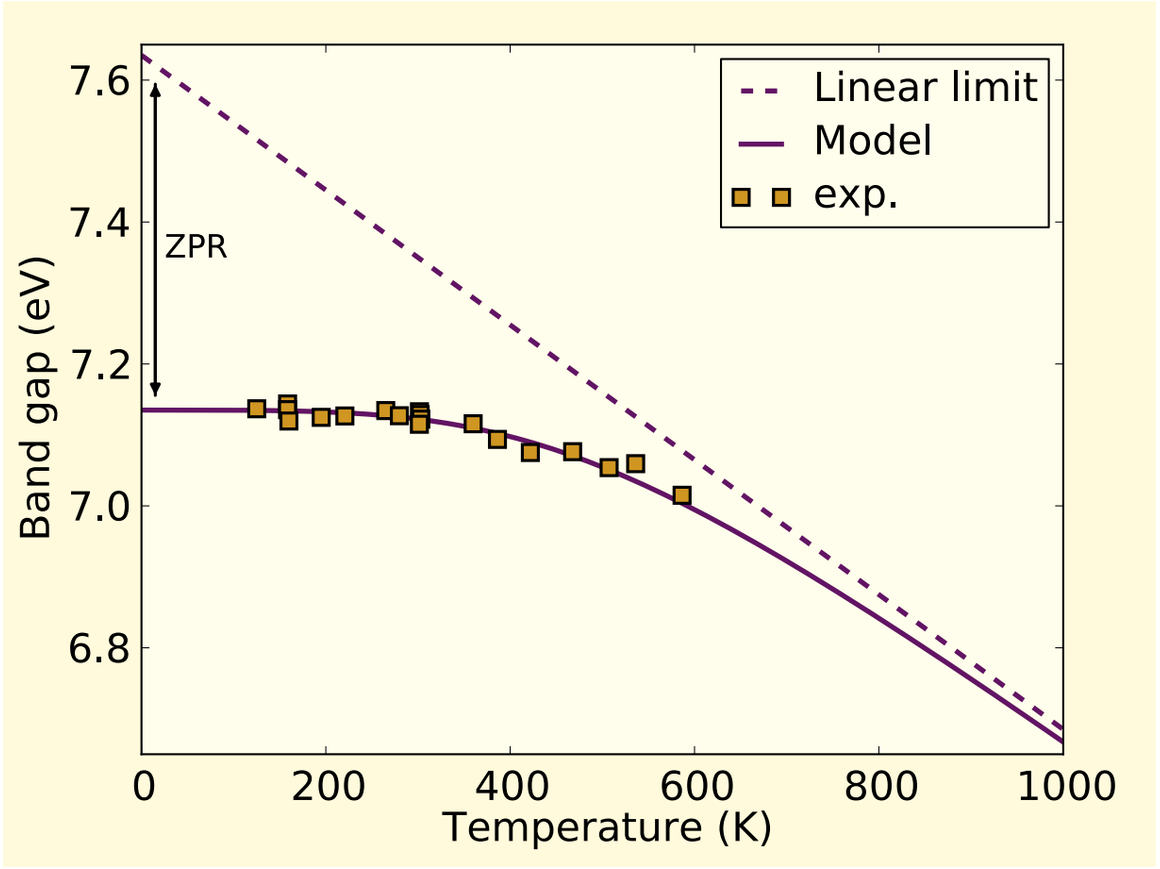
Cons : hard for solids (supercells) ; no anharmonicities ; quadratic ;
adiabatic (vibrations, but no exchange of energy !)

Zero-point renormalization

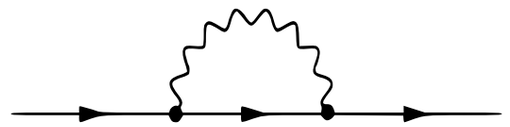


$$\epsilon_\alpha(T) = \epsilon^0_\alpha + \sum_j \frac{\delta\epsilon_\alpha}{\delta n_j} \left[n_j(T) + \frac{1}{2} \right]$$

ZPR



Theory: Allen-Heine-Cardona



$$H = \sum_i^{N_{\rm el}} -\frac{\hbar^2\nabla^2}{2m} + \sum_n^{N_{\rm ion}} -\frac{\hbar^2\nabla^2}{2M_n} + V_{\rm el-el} + V_{\rm ion-ion} + V_{\rm el-ion}$$

$$V_{\rm el-ion} \rightarrow V_{\rm ion}\left(R_n - r_i\right) = V_{\rm ion}\left(R_n^o + \Delta R_n - r_i\right)$$

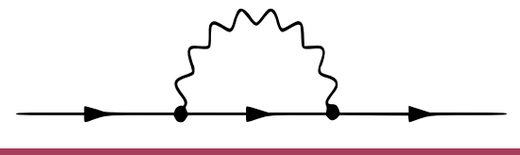
$$= V_{\rm ion}\left(R_n^o - r_i\right) + \nabla V_{\rm ion}\cdot\Delta R_n$$

$$H = E_{\rm el}\left(\{R_n^o\}\right) + \sum_n^{N_{\rm ion}} -\frac{\hbar^2\nabla^2}{2M_n} + V_{\rm ion-ion} + \nabla V_{\rm ion}\cdot\Delta R_n$$

$$H = H_{\rm el} + H_{\rm ion} + \nabla V_{\rm ion}\cdot\Delta R_n$$

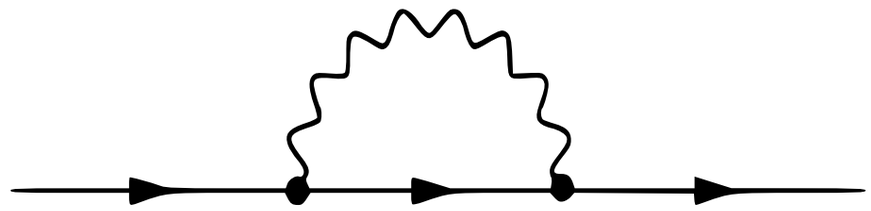
$$H = \sum \epsilon_k c_k^\dagger c_k + \sum \hbar\omega_q(n_q + 1/2) + \sum g_{q,k,k'}(a_q + a_{-q}^\dagger)c_{k+q}^\dagger c_k$$

Theory: Allen-Heine-Cardona



$$H = \sum \epsilon_k c_k^\dagger c_k + \sum \hbar\omega_q (n_q + 1/2) + \underbrace{\sum g_{q,k,k'} (a_q + a_{-q}^\dagger) c_{k+q}^\dagger c_k}_{H'}$$

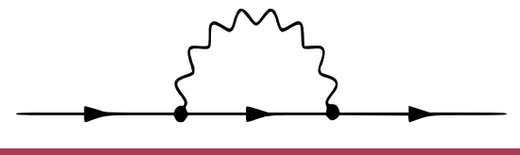
$$\tilde{\epsilon}_k = \epsilon_k + \cancel{\langle \psi_k | H' | \psi_k \rangle} + \sum_{k'} \frac{\langle \psi_k | H' | \psi'_k \rangle \langle \psi'_k | H' | \psi_k \rangle}{\epsilon'_k - \epsilon_k} + \ldots$$

$\tilde{\epsilon}_k = \epsilon_k +$ 

Fan term

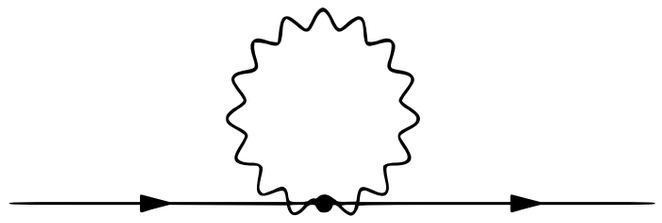
Wait! This is a 2nd order term. We should consider *H*”.

Theory: Allen-Heine-Cardona

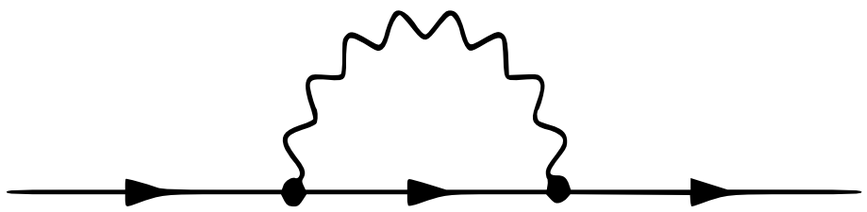


$$V_{\rm ion}\left(R_n - r_i\right) \approx V_{\rm ion}\left(R_n^o - r_i\right) + \nabla V_{\rm ion}\cdot\Delta R_n + \Delta R_{n'}\cdot\nabla\nabla V_{\rm ion}\cdot\Delta R_n$$

H''

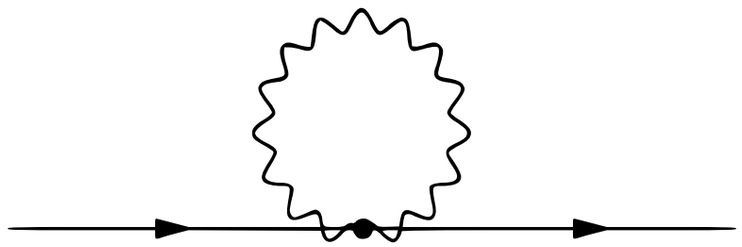


$$\tilde{\epsilon}_k = \epsilon_k +$$



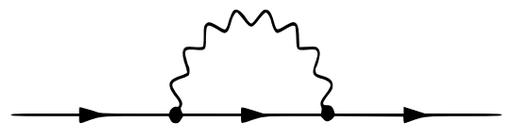
Fan term

$+$



Debye-Waller term

Allen-Heine-Cardona (AHC) formalism



Allen + Heine, J. Phys. C **9, 2305 (1976).** *Allen + Cardona*, Phys. Rev. B **24, 7479 (1981) ; 27, 4760 (1983).**

Second-order (time-dependent) perturbation theory

(no average contribution from first order)

* Formulas for solids (phonons have crystalline momentum)

* If adiabatic BO ... neglect the phonon frequencies with respect to the electronic gap, no transfer of energy :

$$\delta\varepsilon_{\vec{k}n}(T, V = const) = \frac{1}{N_{\vec{q}}} \sum_{\vec{q}j} \frac{\partial \varepsilon_{\vec{k}n}}{\partial n_{\vec{q}j}} \left(n_{\vec{q}j}(T) + \frac{1}{2} \right)$$

occupation number from Bose-Einstein statistics

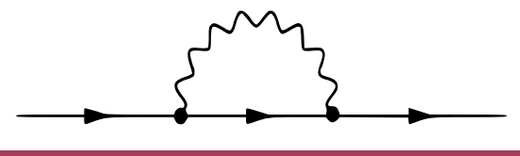
$$\frac{\partial \varepsilon_{\vec{k}n}}{\partial n_{\vec{q}j}} = \frac{1}{2\omega_{\vec{q}j}} \sum_{\kappa a \kappa' b} \frac{\partial^2 \varepsilon_{\vec{k}n}}{\partial R_{\kappa a} \partial R_{\kappa' b}} \frac{\xi_{\kappa a}(\vec{q}j)\xi_{\kappa' b}(-\vec{q}j)}{\sqrt{M_\kappa M_{\kappa'}}} e^{iq.(R_{\kappa' b} - R_{\kappa a})}$$

Electron-phonon coupling energy (EPCE)

"Phonon mode factor"

$\xi_{\kappa a}(\vec{q}j)$ phonon eigenmodes, κ = atom label, a=x, y, or z

Allen-Heine-Cardona (AHC) formalism



$$\left(\frac{\partial^2 \varepsilon_{\vec{k}n}}{\partial R_{\kappa a} \partial R_{\kappa' b}} \right) = ?$$

$$\varepsilon_{\vec{k}n} = \left\langle \phi_{\vec{k}n} \middle| \hat{H}_{\vec{k}} \middle| \phi_{\vec{k}n} \right\rangle \qquad \hat{H} = \hat{T} + \hat{V}_{\text{nucl}} + \int \frac{\rho(r')}{|r-r'|} dr' + \frac{dE_{xc}}{d\rho(r)}$$

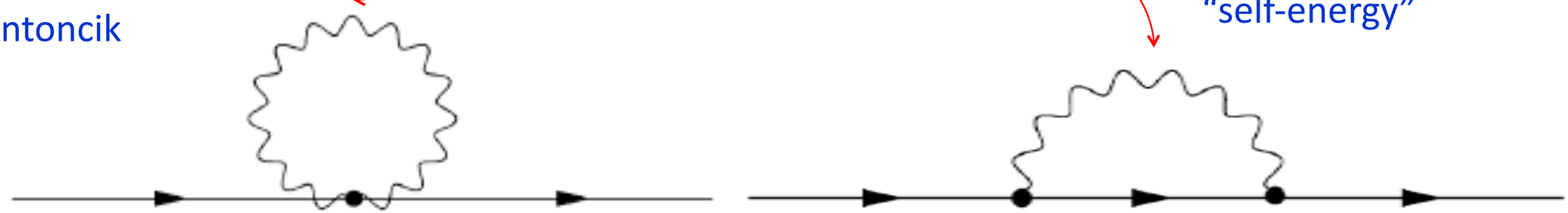
Hellman-Feynman theorem : $$\varepsilon^{(1)}_{\vec{k}n} = \left\langle \phi^{(0)}_{\vec{k}n} \middle| \hat{H}^{(1)}_{\vec{k}} \middle| \phi^{(0)}_{\vec{k}n} \right\rangle$$

One more derivative :

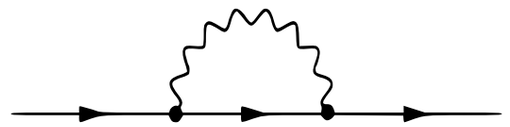
$$\varepsilon^{(2)}_{\vec{k}n} = \left\langle \phi^{(0)}_{\vec{k}n} \middle| \hat{H}^{(2)}_{\vec{k}} \middle| \phi^{(0)}_{\vec{k}n} \right\rangle + \frac{1}{2}\left(\left\langle \phi^{(0)}_{\vec{k}n} \middle| \hat{H}^{(1)}_{\vec{k}+\vec{q}} \middle| \phi^{(1)}_{\vec{k}\vec{q}n} \right\rangle + (c.c) \right)$$

Debye-Waller
Antoncik

Fan
“self-energy”

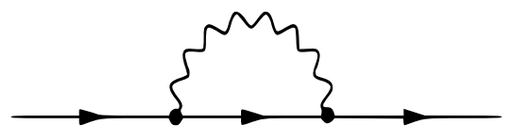


Outline



- Introduction/Motivations
- Theory: Allen-Heine-Cardona
- Calculations for diamond
  - at the density-functional theory level
  - at the GW method level
  - including anharmonic effects
  - including dynamical effects
- Conclusion

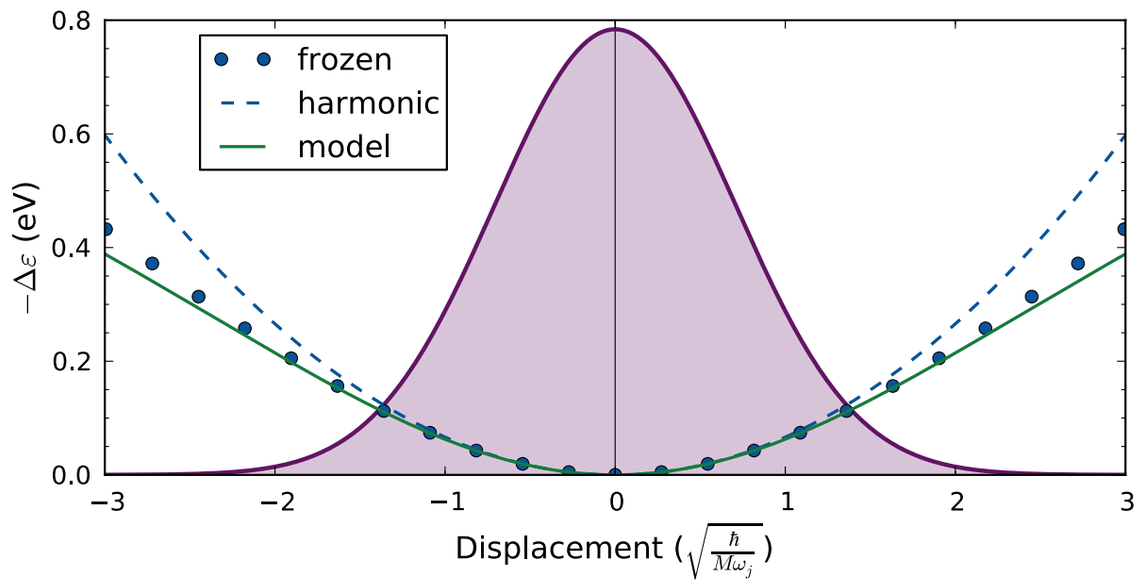
Evaluation of matrix elements



Choose an electronic structure method.

Frozen-phonon method:

$$\frac{\partial \varepsilon_\alpha}{\partial n_j} = \frac{\hbar}{2M\omega_j}\frac{\partial^2}{\partial z^2}\varepsilon_\alpha\left[z\mathbf{u}_\tau^j\right]\Big|_{z=0}$$

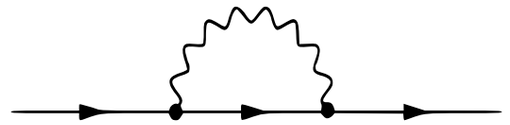


Direct approach with perturbation theory:

$$\frac{\partial \varepsilon_\alpha}{\partial n_j} = \frac{\hbar}{2M\omega_j}\sum_{\tau,\tau'}\Phi^\alpha_{\tau,\tau'} : \left[\mathbf{u}_\tau^{j\dagger}\mathbf{u}_{\tau'}^j - \frac{1}{2}\left(\mathbf{u}_\tau^{j\dagger}\mathbf{u}_\tau^j + \mathbf{u}_{\tau'}^{j\dagger}\mathbf{u}_{\tau'}^j\right)\right]$$

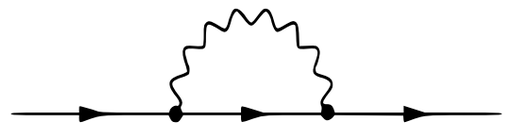
$$\Phi^\alpha_{\tau,\tau'} = \left(\langle\psi_\alpha|\nabla_\tau H|\nabla_{\tau'}\psi_\alpha\rangle + \text{c.c.}\right) + \langle\psi_\alpha|\nabla_\tau\nabla_{\tau'}H|\psi_\alpha\rangle$$

Evaluation of matrix elements



- Use density-functional theory in the LDA approximation
- Calculate phonons using density-functional perturbation theory (DFPT)
- Matrix elements evaluation
  - Directly by frozen-phonon
  - Calculated using DFPT

Numerical study : ZPR in diamond



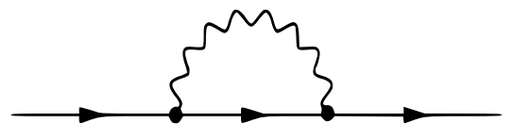
-Implementation in ABINIT (www.abinit.org)
-Plane wave + pseudopotential methodology
-Converged number of plane waves (30 ... 40 Hartree)
-k point sampling : 6x6x6 sufficient for first-order Hamiltonian
-Density Functional Perturbation Theory for phonons => no sum on conduction bands, no supercell need ; reformulation of the Debye-Waller term thanks to the rigid-ion approximation
-Sampling on the q phonon wavevectors for the Fan term is a big issue !

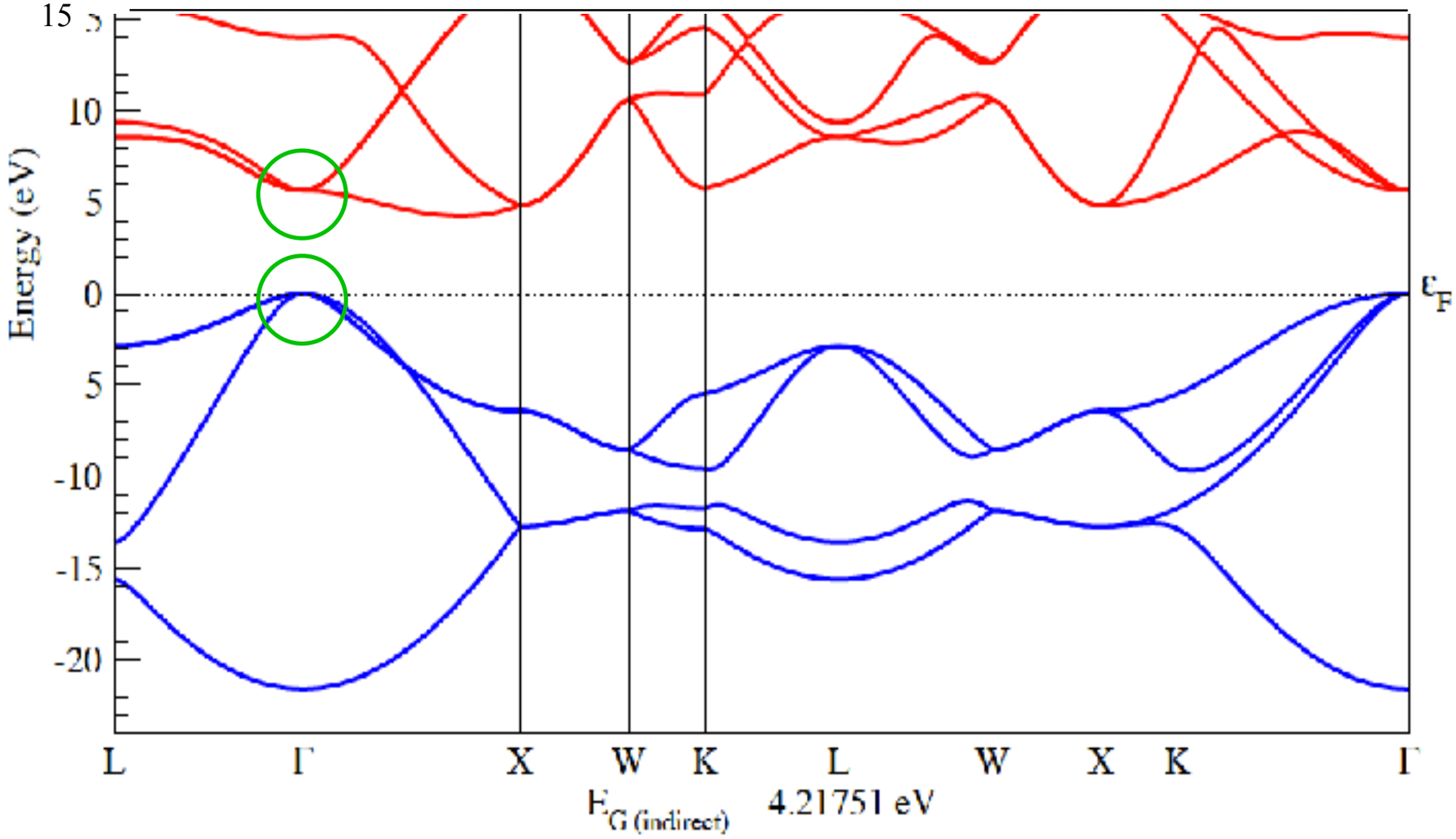
$$\delta\varepsilon_{\Gamma n}^{ZPM} = \frac{1}{N_{\vec{q}}}\sum_{\vec{q}j}\frac{\partial\varepsilon_{\Gamma n}}{\partial n_{\vec{q}j}}\frac{1}{2}$$

$$\frac{\partial\varepsilon_{\Gamma n}(Fan)}{\partial n_{\vec{q}j}} = \frac{1}{\omega_{\vec{q}j}}\Re\sum_{\kappa a\kappa' bn'}\frac{\left\langle\phi_{\Gamma n}\left|\nabla_{\kappa a}H_{\kappa}\right|\phi_{\vec{q}n'}\right\rangle\left\langle\phi_{\vec{q}n'}\left|\nabla_{\kappa' b}H_{\kappa'}\right|\phi_{\Gamma n}\right\rangle}{\varepsilon_{\Gamma n}-\varepsilon_{\vec{q}n'}}\frac{\xi_{\kappa a}(\vec{q}j)\xi_{\kappa' b}(-\vec{q}j)}{\sqrt{M_{\kappa}M_{\kappa'}}}e^{iq.(R_{\kappa' b}-R_{\kappa a})}$$

Indeed intraband contributions diverge due to the denominator !
Still, can be integrated out … for diamond ...

Intraband divergence for small q





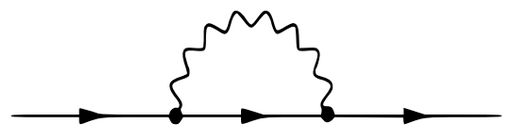
$$\lim_{\vec{q}\to 0}\frac{\partial \varepsilon_{\Gamma n}(Fan)}{\partial n_{\vec{q}j}} = \lim_{\vec{q}\to 0}\frac{1}{\omega_{\vec{q}j}}\frac{f(\vec{q}jn)}{\varepsilon_{\Gamma n}-\varepsilon_{\vec{q}n}}$$

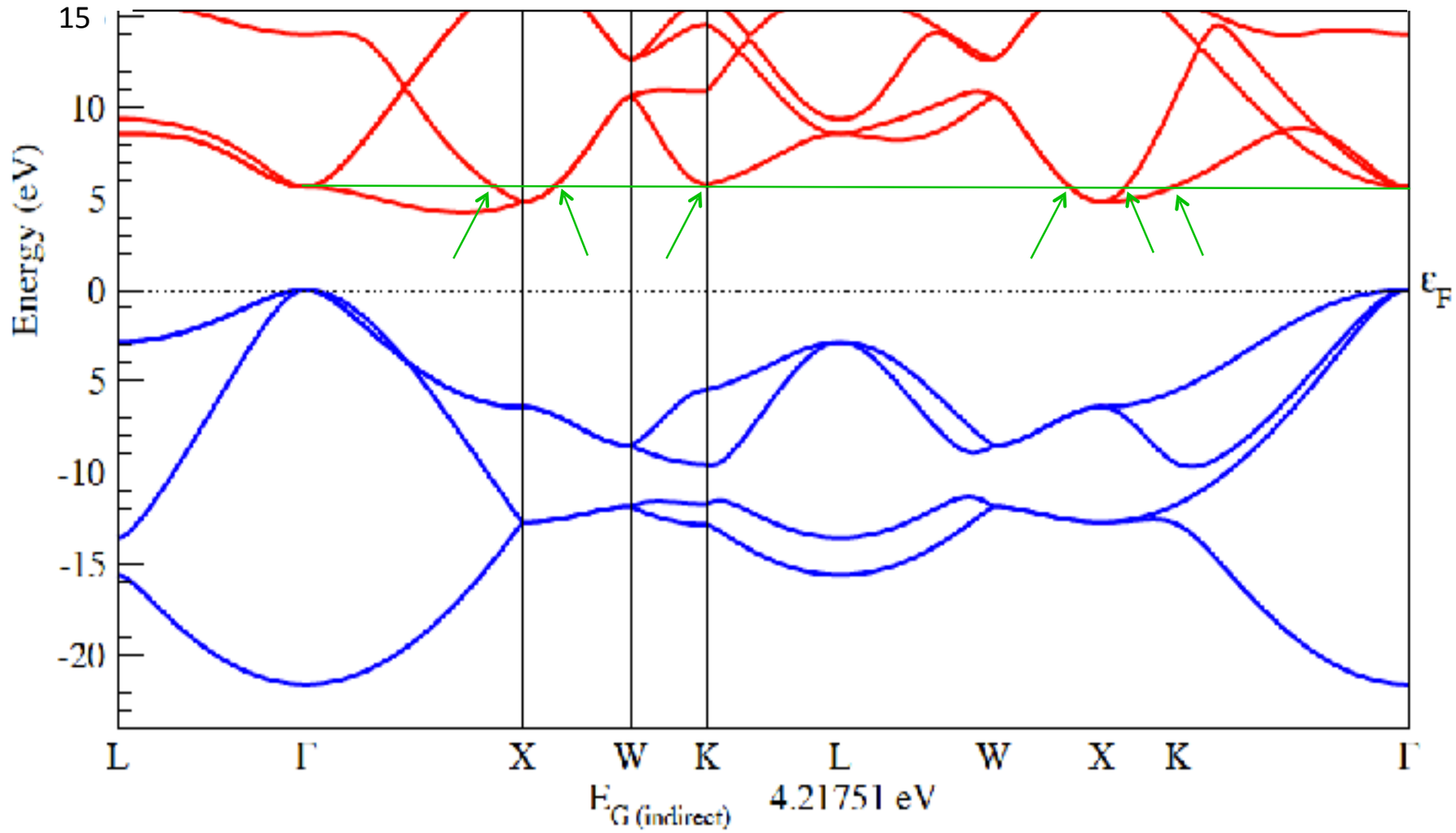
Optic modes : $\lim_{\vec{q}\to 0}\frac{\partial \varepsilon_{\Gamma n}(Fan)}{\partial n_{\vec{q}j}} \propto \frac{1}{q^2}$

Can be integrated in 3D !

+ For acoustic modes, Fan/DDW contribs cancel each other

Divergences on isoenergetic surface





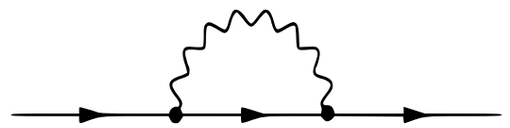
Set of isoenergetic wavevectors

$$\lim_{\vec{q}\to\vec{q}_{iso}} \frac{\partial \varepsilon_{\Gamma n}(Fan)}{\partial n_{\vec{q}j}} = \lim_{\vec{q}\to\vec{q}_{iso}} \frac{1}{\omega_{\vec{q}j}} \frac{f(\vec{q}jn)}{\varepsilon_{\Gamma n} - \varepsilon_{\vec{q}n}} \propto \frac{1}{\nabla_{\vec{q}} \varepsilon_{\vec{q}n}\Big|_{\vec{q}_{iso}} .(\vec{q} - \vec{q}_{iso})}$$

Can be integrated !

Such problem occurs only off the extrema

Smoothing the denominator



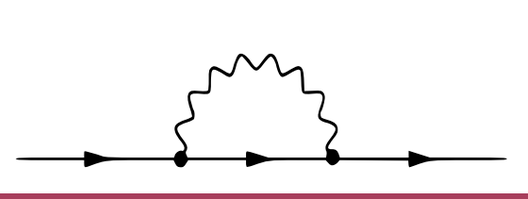
$$\frac{\partial \varepsilon_{\Gamma n}(Fan)}{\partial n_{\vec{q}j}} = \frac{1}{\omega_{\vec{q}j}} \Re \sum_{\kappa a \kappa' b n'} \frac{\left\langle \phi_{\Gamma n} \middle| \nabla_{\kappa a} H_{\kappa} \middle| \phi_{\vec{q}n'} \right\rangle \left\langle \phi_{\vec{q}n'} \middle| \nabla_{\kappa' b} H_{\kappa'} \middle| \phi_{\Gamma n} \right\rangle}{\varepsilon_{\Gamma n} - \varepsilon_{\vec{q}n'} + i\delta} \frac{\xi_{\kappa a}(\vec{q}j)\xi_{\kappa' b}(-\vec{q}j)}{\sqrt{M_{\kappa} M_{\kappa'}}} e^{iq.(R_{\kappa' b} - R_{\kappa a})}$$

... dramatically helps the convergence … to a (slightly) different value …

If imaginary part = 100 meV (considering direct gap at Gamma) :

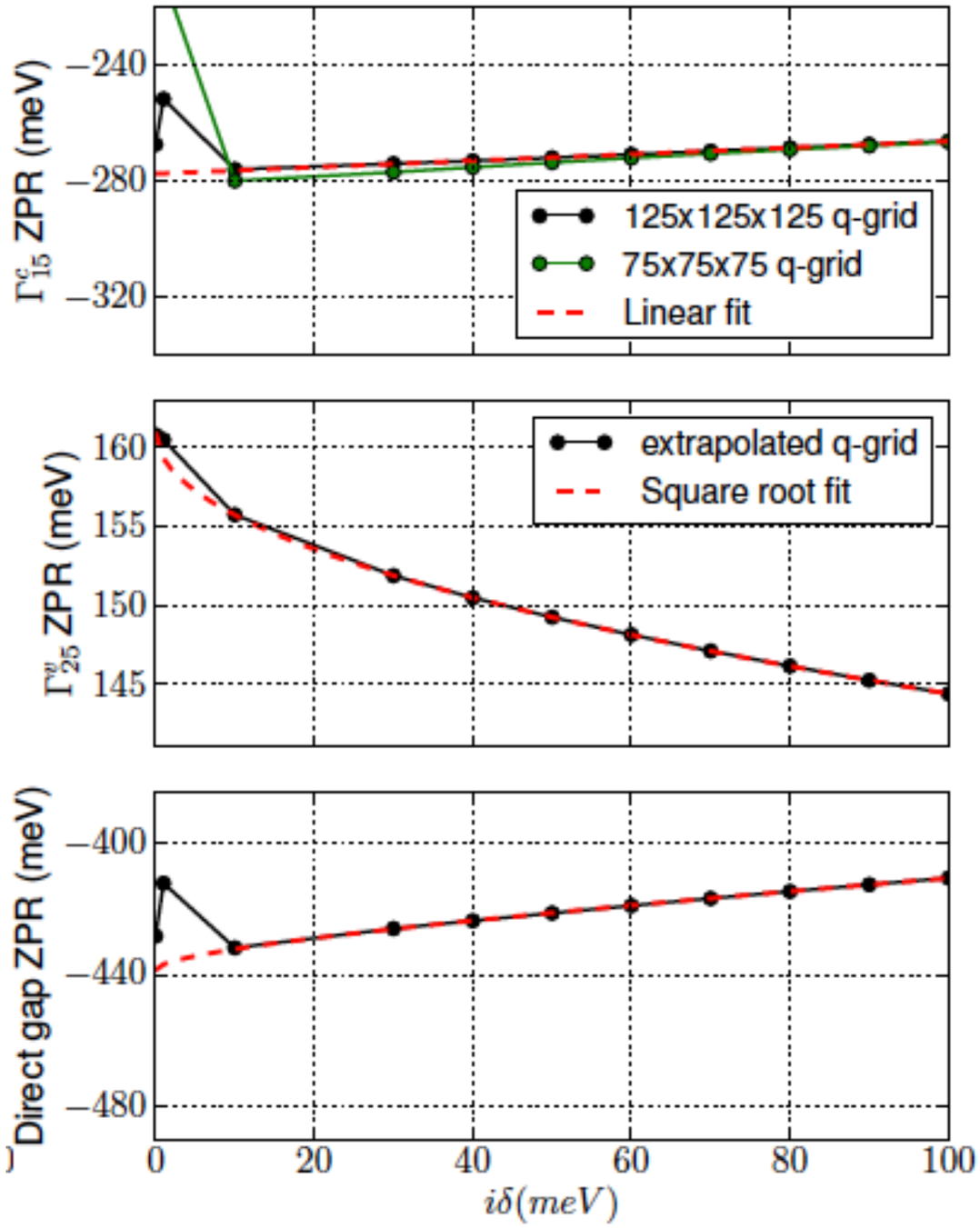
q grid	#q in IBZ	ZPR VBM (meV)	ZPR CBM (meV)	ZPR gap (meV)
8x8x8 x4s	60	140.5	-181.9	-322.4
12x12x12 x4s	182	141.7	-293.1	-434.8
16x16x16 x4s	408	141.7	-273.9	-415.6
20x20x20 x4s	770	141.7	-260.1	-401.8
24x24x24 x4s	1300	141.7	-257.5	-399.2
28x28x28 x4s	2030	141.7	-269.1	-410.8
32x32x32 x4s	2992	141.7	-271.8	-413.5

Changing the imaginary delta

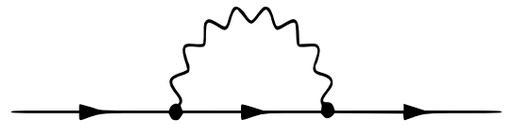


$$\frac{f(\vec{q}jn)}{\varepsilon_{\Gamma n} - \varepsilon_{\vec{q}n} + i\delta}$$

For very large q-wavevector sampling, …
rate of convergence understood,
+ correspond to expectations !



Cross-checking

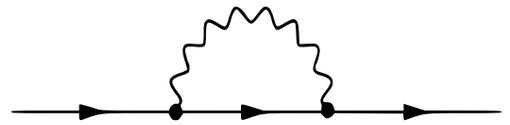


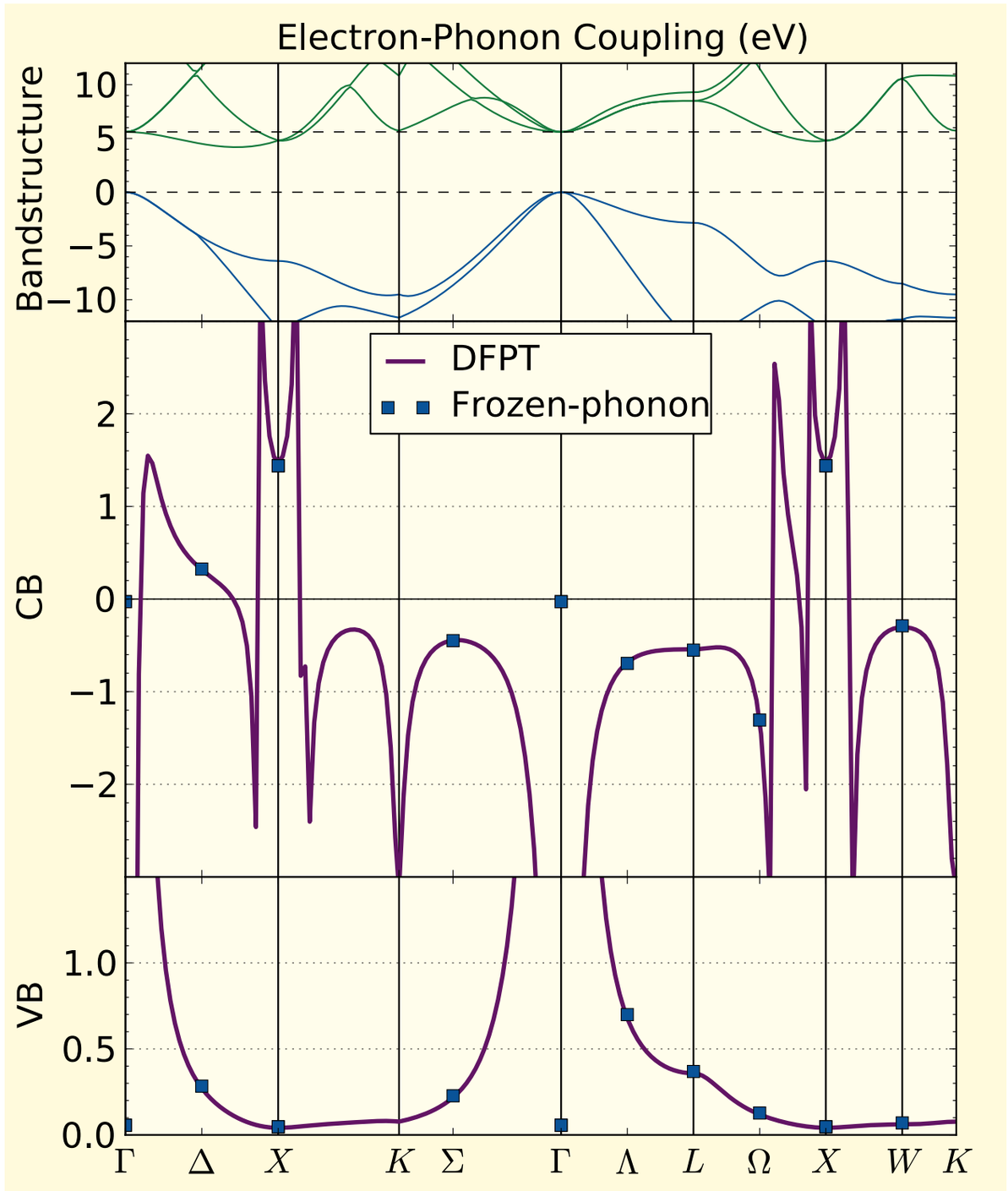
Independent implementation in Quantum-Espresso + Yambo
=> excellent agreement with ABINIT … 0.4 eV

Band	Fan + DDW	
	ABINIT 7.3.2 SEq/ 300 bands	Yambo 3.4.0 300 bands
1	−61.75	−61.87
2–3–4	140.54	140.70
5–6–7	−260.63	−259.40
8	−232.37	−230.40
9	−43.86	−43.95
ZPR Band gap	-401.17 meV	-400.10 meV

S. Poncé *et al, Comput. Materials Science* 83, 341 (2014)

DFTP vs Frozen-phonon





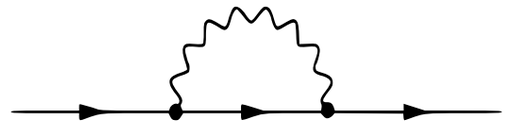
$$\frac{\delta \epsilon_\alpha}{\delta n_j}$$

ZPR (meV)

	VB	CB	Gap
DFPT	113	-314	-427
Frozen-phonon	117	-320	-437
Exp.			~-600

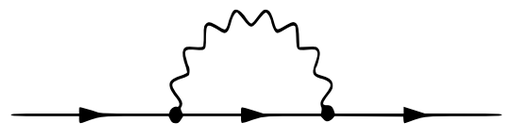
equivalent q-points

- Good agreement between different approaches
- Still large difference with experimental value



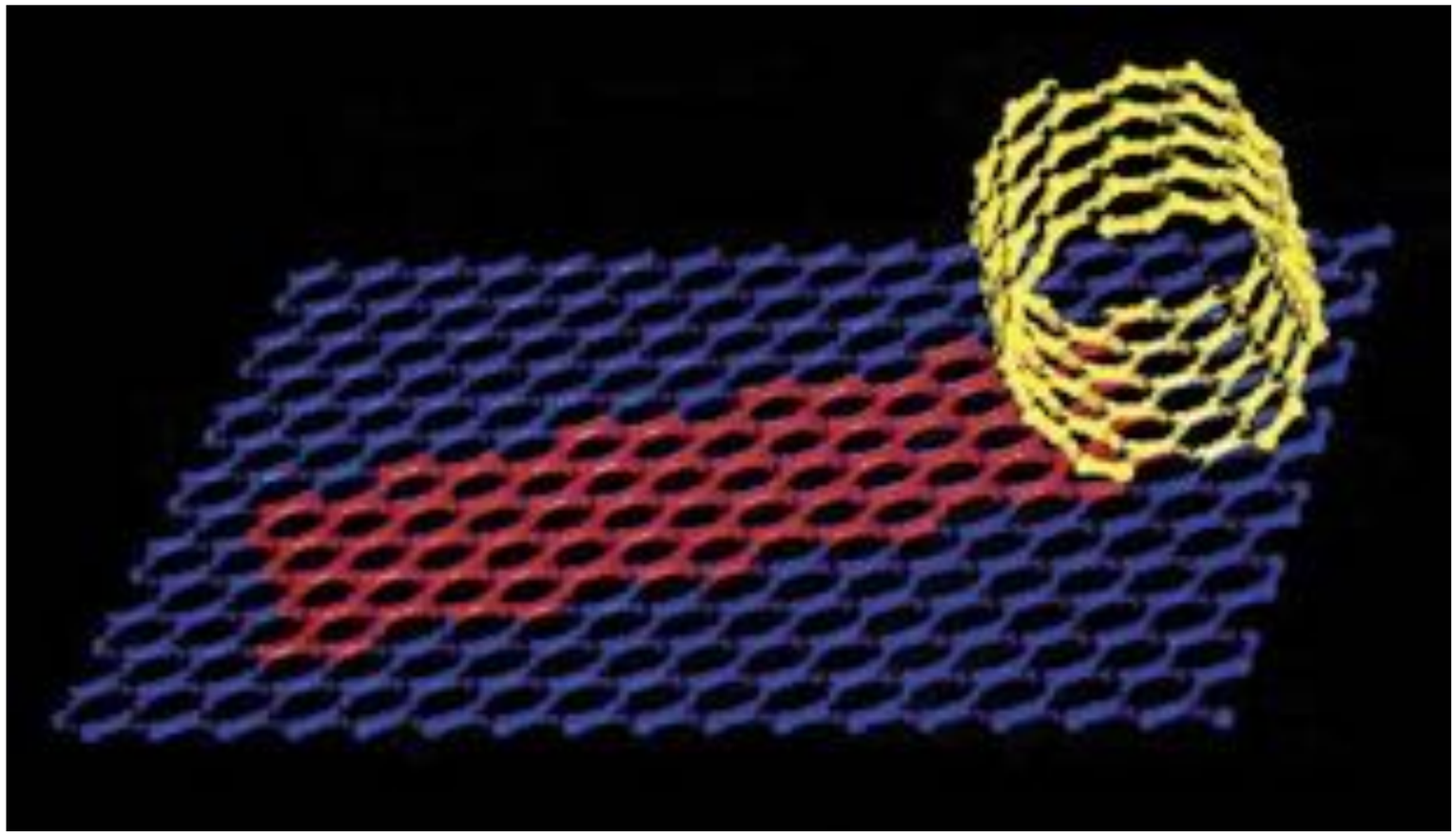
Is LDA enough…

Nanotubes



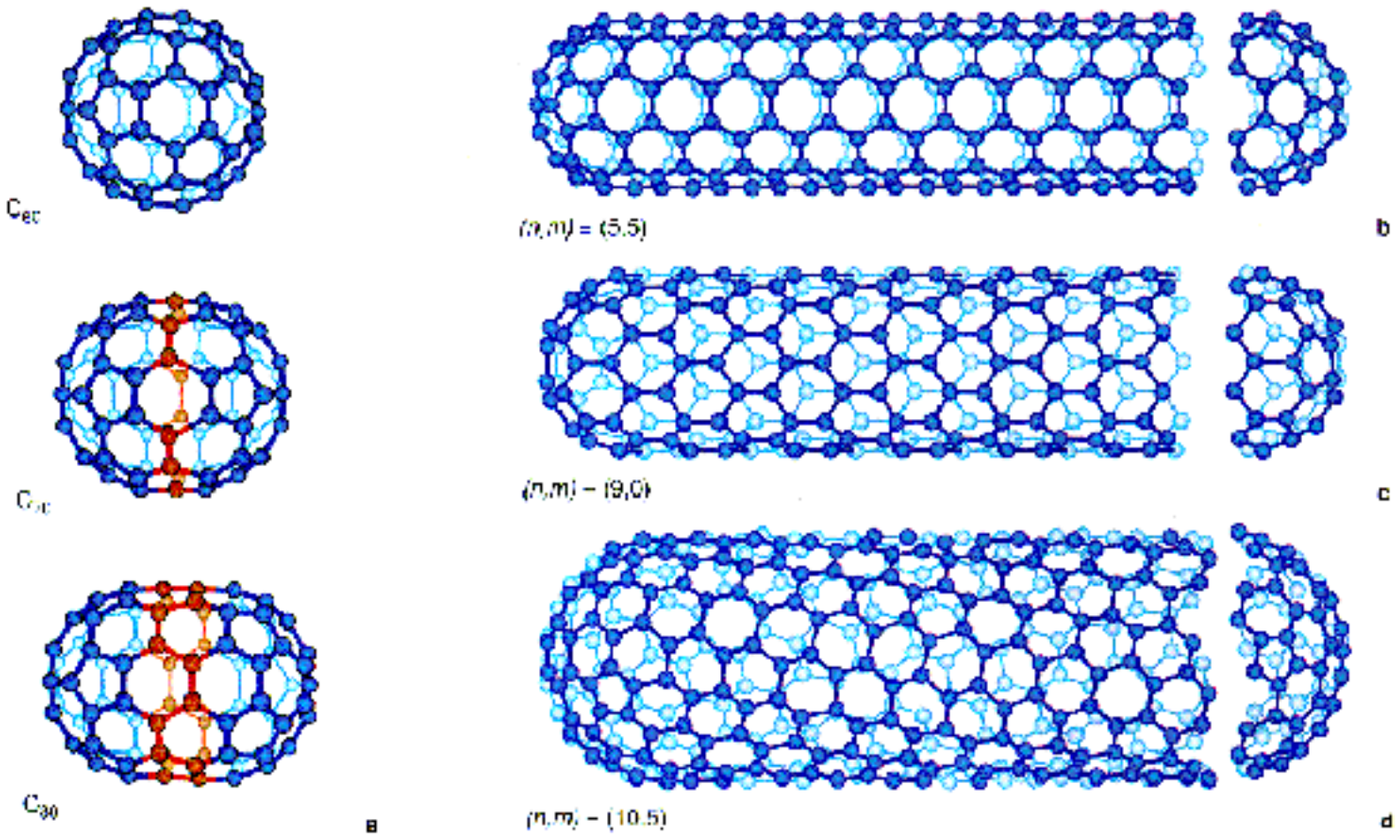

ADVANCED MATERIALS
nature
Science
Science Journal
Carbon Nanotubes
1991
2001
The First Ten Years
nature
www.naturejpn.com
American Scientist
Science
1 February 2002
Up close to nanotube wavefunctions
Guardian of the genome Structure of Ku/DNA complex
Carbene chemistry The elusive triplet trapped
EPO signalling Protection from brain ischaemia
Ageing
Building immunity
The T-cell repertoire

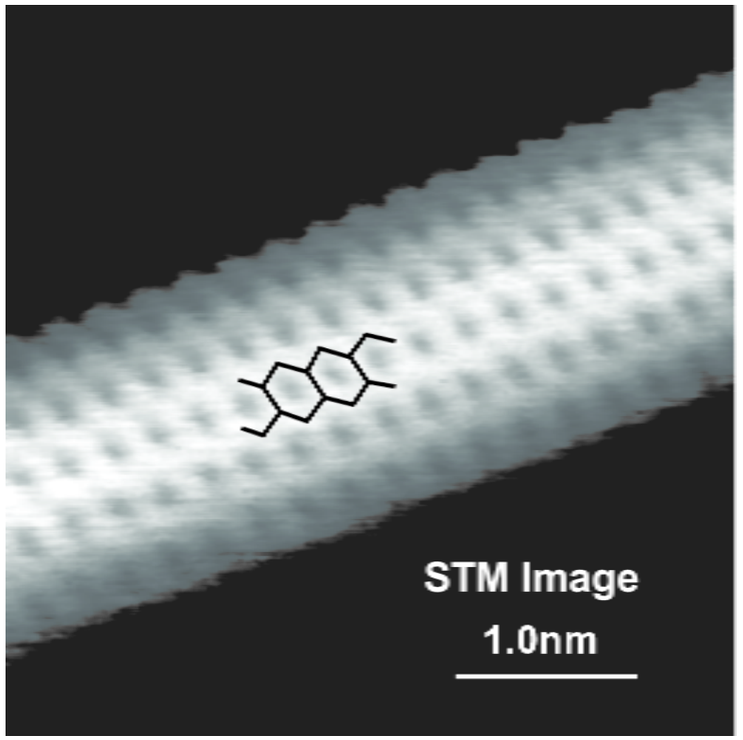
How to form a nanotube



- A nanotube is a roll up graphene sheet

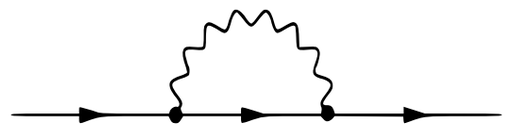
Nanotubes as long fullerenes





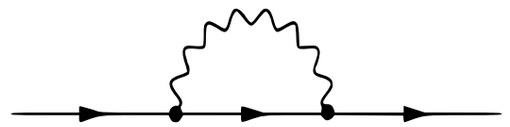
Dresselhaus, Dresselhaus & Eklund. 1996 Science of Fullerenes and Carbon Nanotubes. San Diego, Academic Press.

Long soccer ball



Ref: Laurent Perbos

Metallic nanotubes



According to Peierls, 1D conductors are unstable below a certain temperature at which a electronic gap will open. This is similar to mechanism of Jahn-Teller effect for finite systems.

VOLUME 68, NUMBER 5 PHYSICAL REVIEW LETTERS 3 FEBRUARY 1992

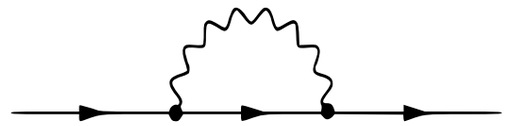
Are Fullerene Tubules Metallic?

J. W. Mintmire, B. I. Dunlap, and C. T. White
Naval Research Laboratory, Washington, DC 20375-5000
(Received 9 October 1991)

We have calculated the electronic structure of a fullerene tubule using a first-principles, self-consistent, all-electron Gaussian-orbital based local-density-functional approach. Extending these results to a model containing an electron-lattice interaction, we estimate that the mean-field transition temperature from a Peierls-distorted regime to a high-temperature metallic regime should be well below room temperature. Such fullerene tubules should have the advantages (compared to other conjugated carbon systems) of a carrier density similar to that of metals and zero band gap at room temperature.

PACS numbers: 71.20.Hk, 31.20.Sy, 36.20.Kd, 72.80.Le

Peierls and response function



Linear response of a system:

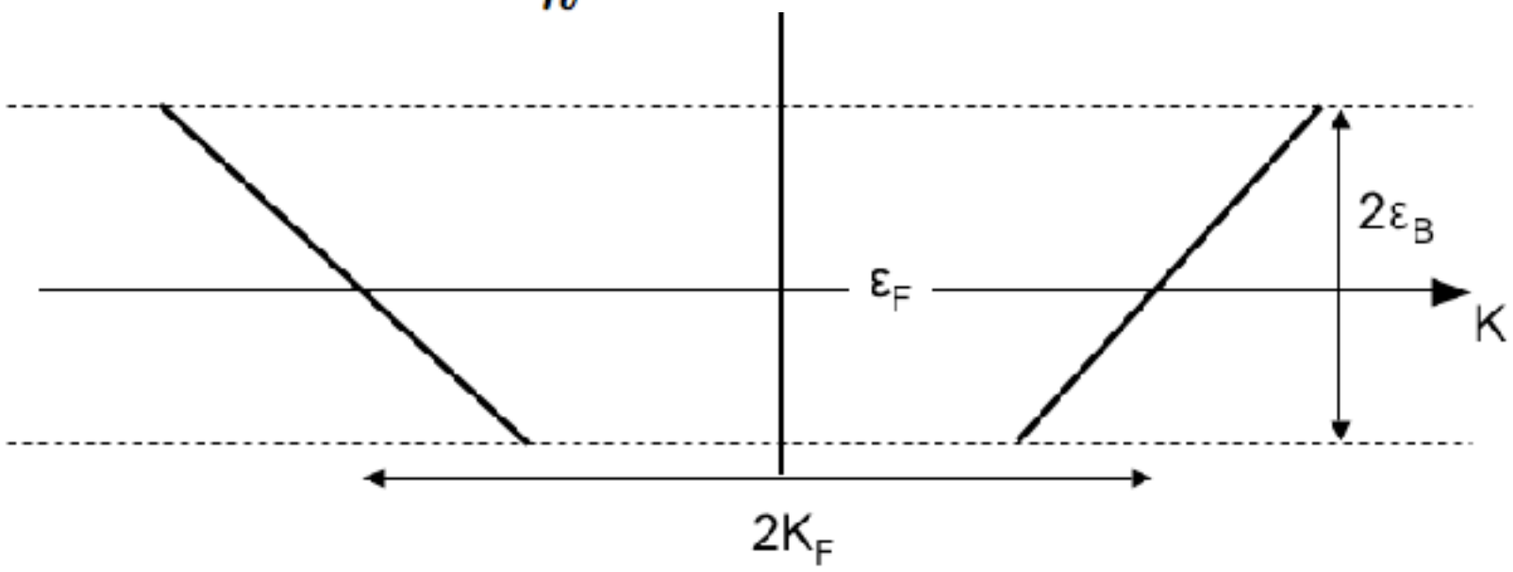
$$\delta n(r) = \int dr' \chi(r - r') \delta v(r')$$

$$\delta n(Q) = \chi(Q) \delta v(Q)$$

For non-interacting electrons, we have:

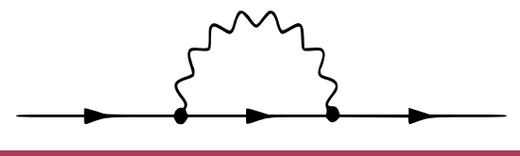
$$\chi(Q) = \frac{2}{N} \sum_k \frac{f_k - f_{k+Q}}{\epsilon_k - \epsilon_{k+Q}}$$

$$f_k = \frac{1}{e^{\frac{\epsilon_k}{k_B T}} + 1}$$



$$\epsilon_k = V_F \hbar (|k| - k_F)$$

Peierls and response function (2)

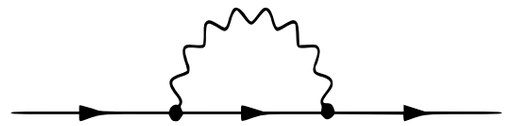


$$\chi(2k_F) = \frac{a}{\pi}\int_{k(-\epsilon_B)}^{k(\epsilon_B)} dk \frac{f(\epsilon_k) - f(-\epsilon_k)}{2\epsilon_k}$$

$$\begin{aligned}\chi(2k_F, T) &= -\frac{a}{\pi\hbar V_F}\int_0^{\epsilon_B} \frac{d\epsilon}{\epsilon}\tanh(\frac{\epsilon}{2k_BT}) \\ &= -\frac{a}{\pi\hbar V_F}\ln\left[\frac{1,13\epsilon_B}{k_BT}\right]\end{aligned}$$

For T=0, the response of the system is negative and infinite.

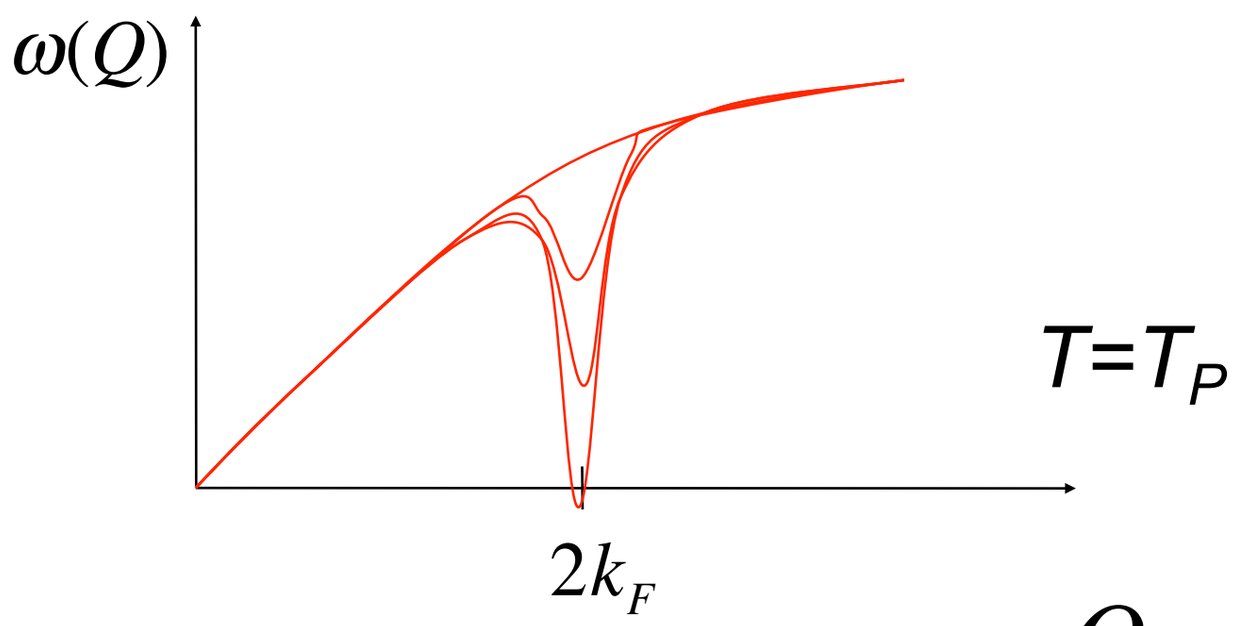
Phonons in 1D metal



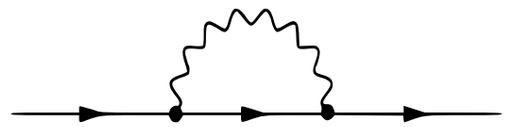
$$H_{e-p} = \frac{1}{\sqrt{N}} \sum_Q g(Q) u(Q) n_{-Q}$$

$$\omega^2(Q) = \omega_0^2(Q) \left[1 + \left(2 \frac{2g^2(Q)}{\hbar \omega_0(Q)} \right) \chi(Q,T) \right]$$

$$k_B T_P = 1.13 \epsilon_B e^{\frac{-\pi \hbar^2 V_F \omega_0(2k_F)}{2a g^2(2k_F)}}$$

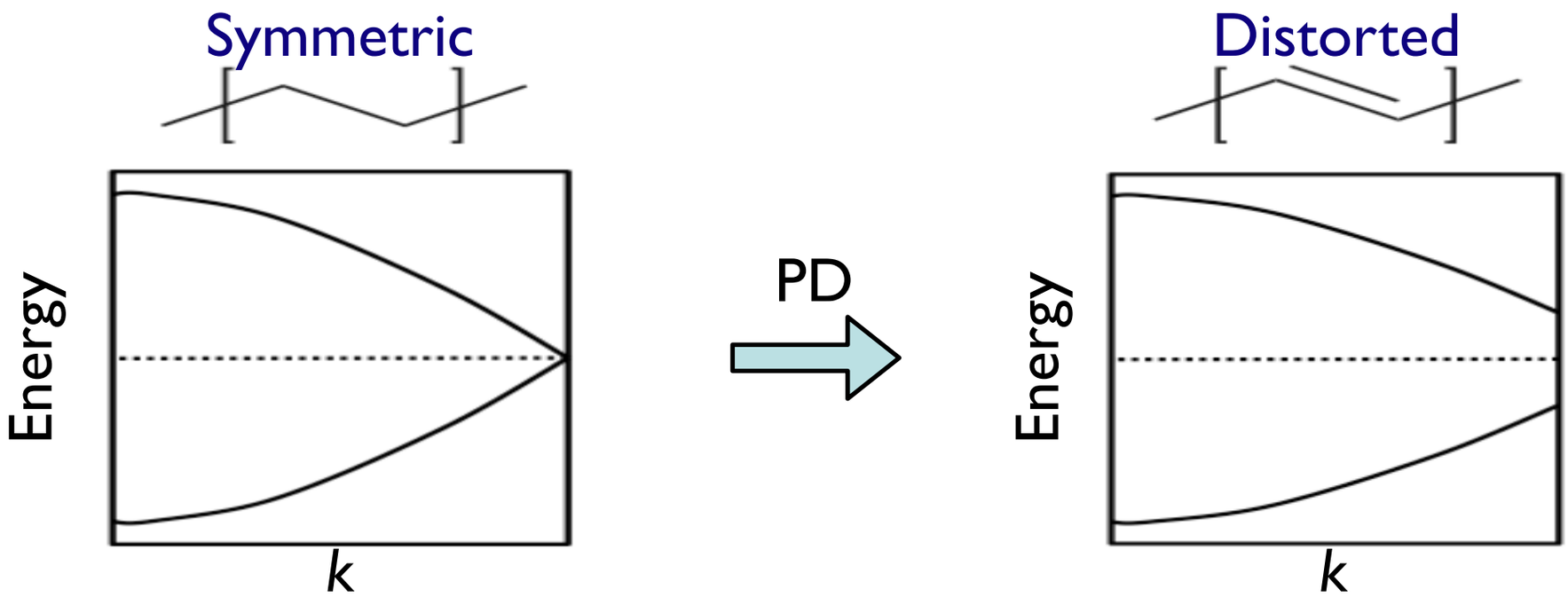


Peierls distortion

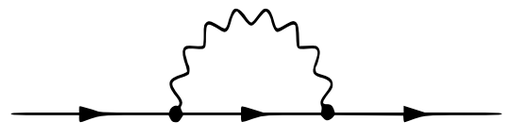


A Peierls distortion (PD) lowers the energy of a system by lowering its symmetry. This mechanism is mediated by a phonon of a given wave-vector *q*.

Polyacetylene



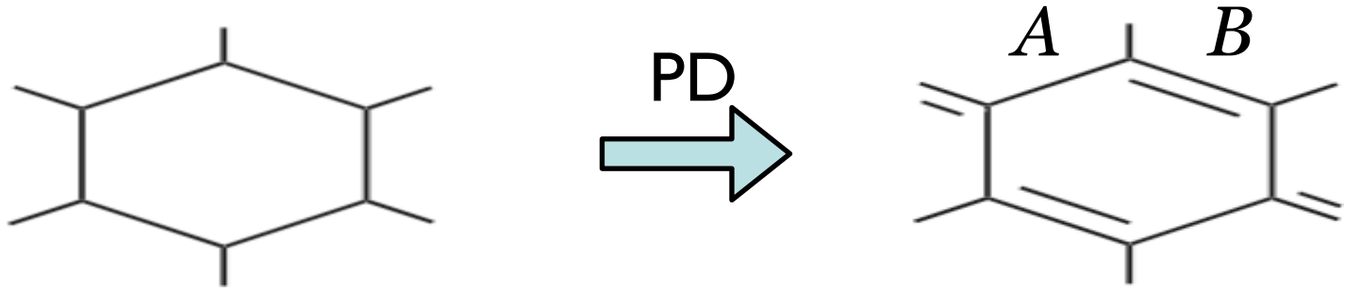
Functionals



- Usual LDA or GGA functionals cannot reproduce the correct geometry of polyacetylene
- Hybrid functionals, including HF exchange, such as B3LYP can
- Find the functional that reproduce the geometry of polyacetylene
- Apply this functional to CNTs ⇒ observe PD

$$E_{XC} = (1-x)(E_X^{\text{Slater}} + \Delta E_X^{\text{PBE}}) + xE_X^{\text{HF}} + E_C^{\text{PBE}}$$

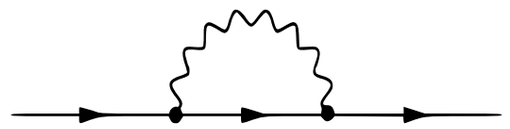
Type of distortion

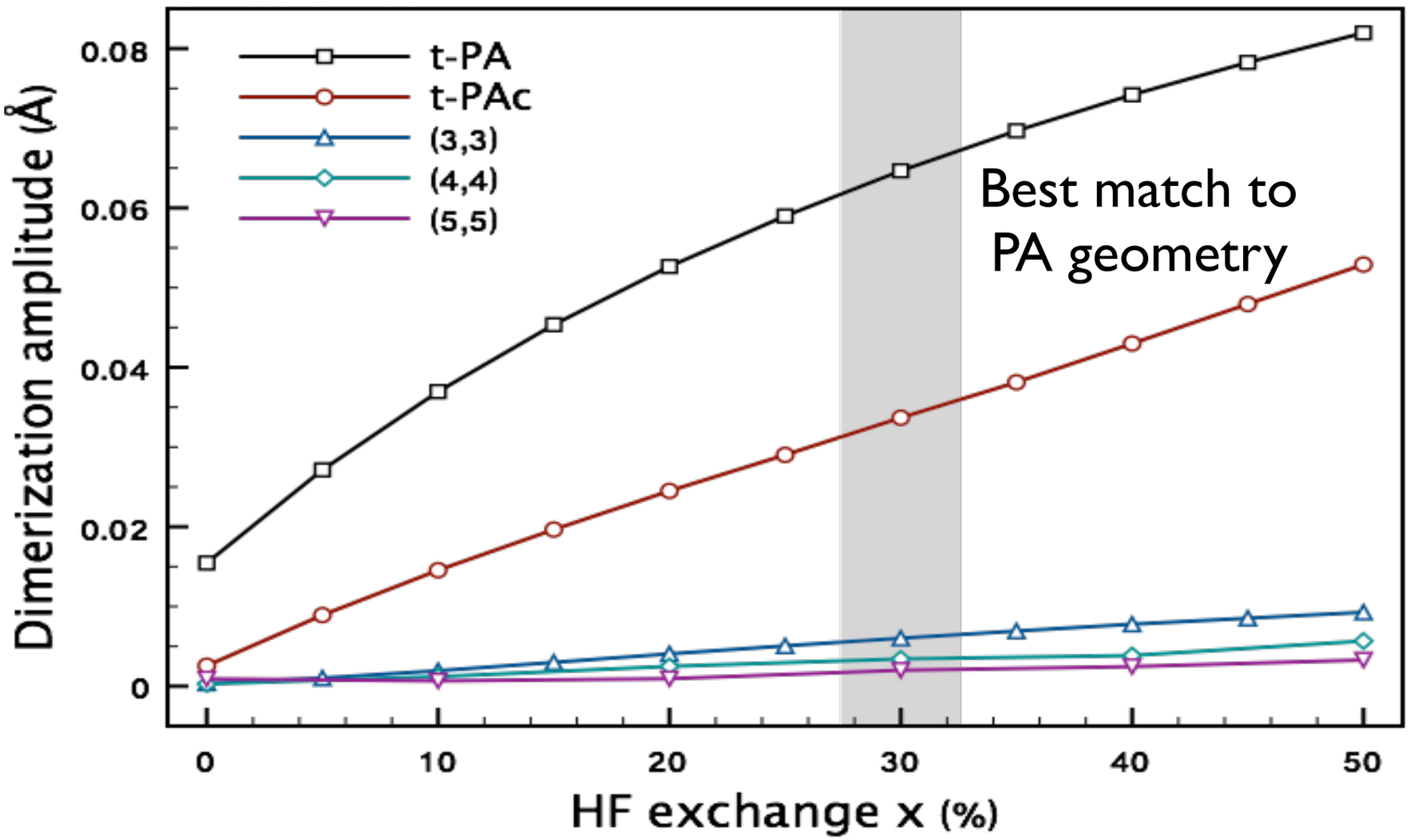


q = 0,
since we use only one unit cell

- Dimerization amplitude = Bond length alternation (BLA) = *A* - *B*
- Hartree-Fock exchange = Exact exchange

Polyacetylene

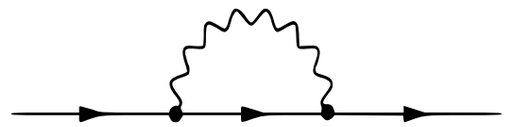


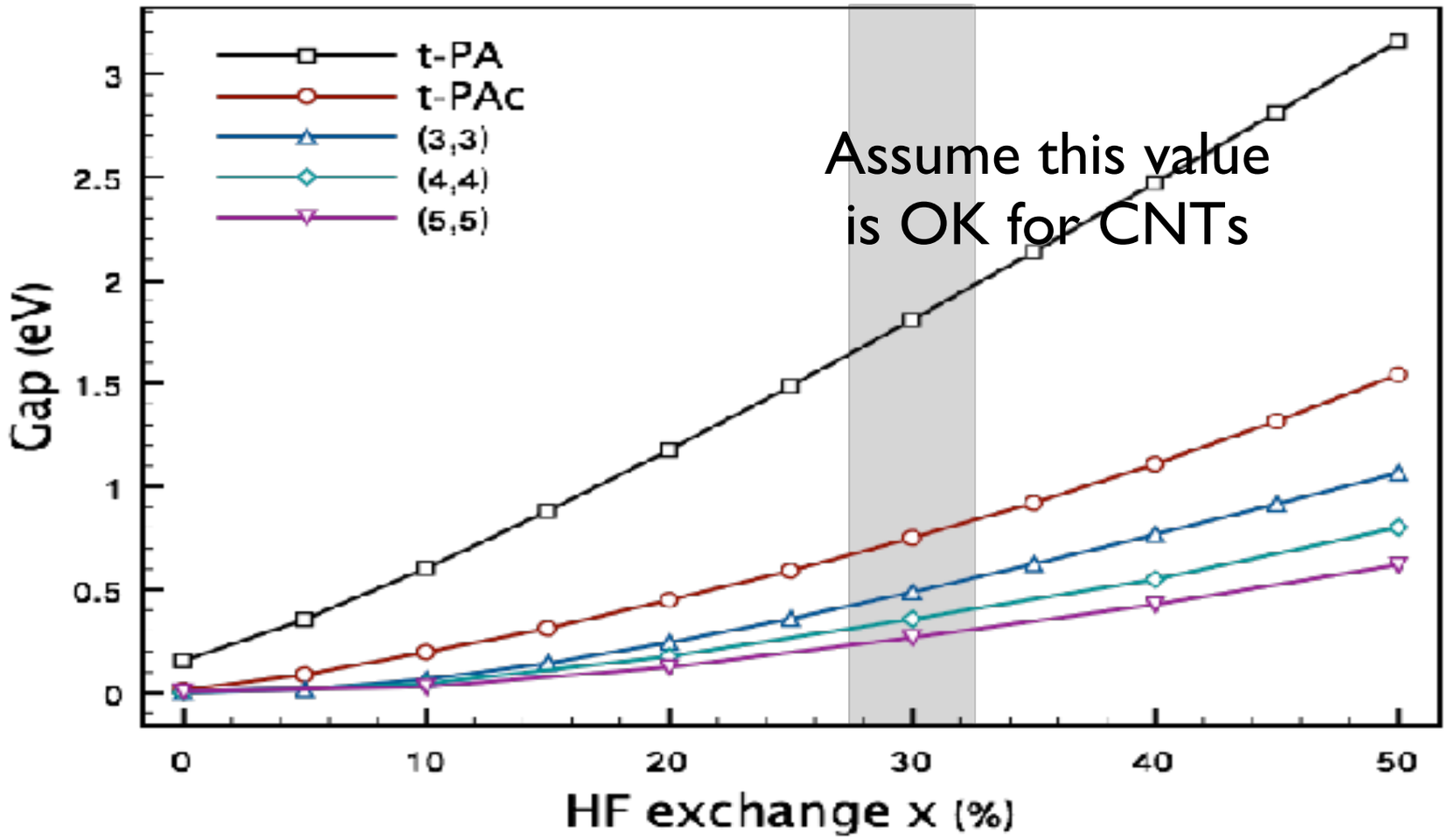


Values of bond lengths and band gap of PA

Qty	EXP	x = 0.0	B3LYP	x = 0.3
C–C (Å)	1.44	1.41	1.43	1.43
C=C (Å)	1.36	1.40	1.47	1.36
Gap (eV)	1.50	0.16	1.25	1.81

x = 0.3 gives the best agreement





Assume this value is OK for CNTs

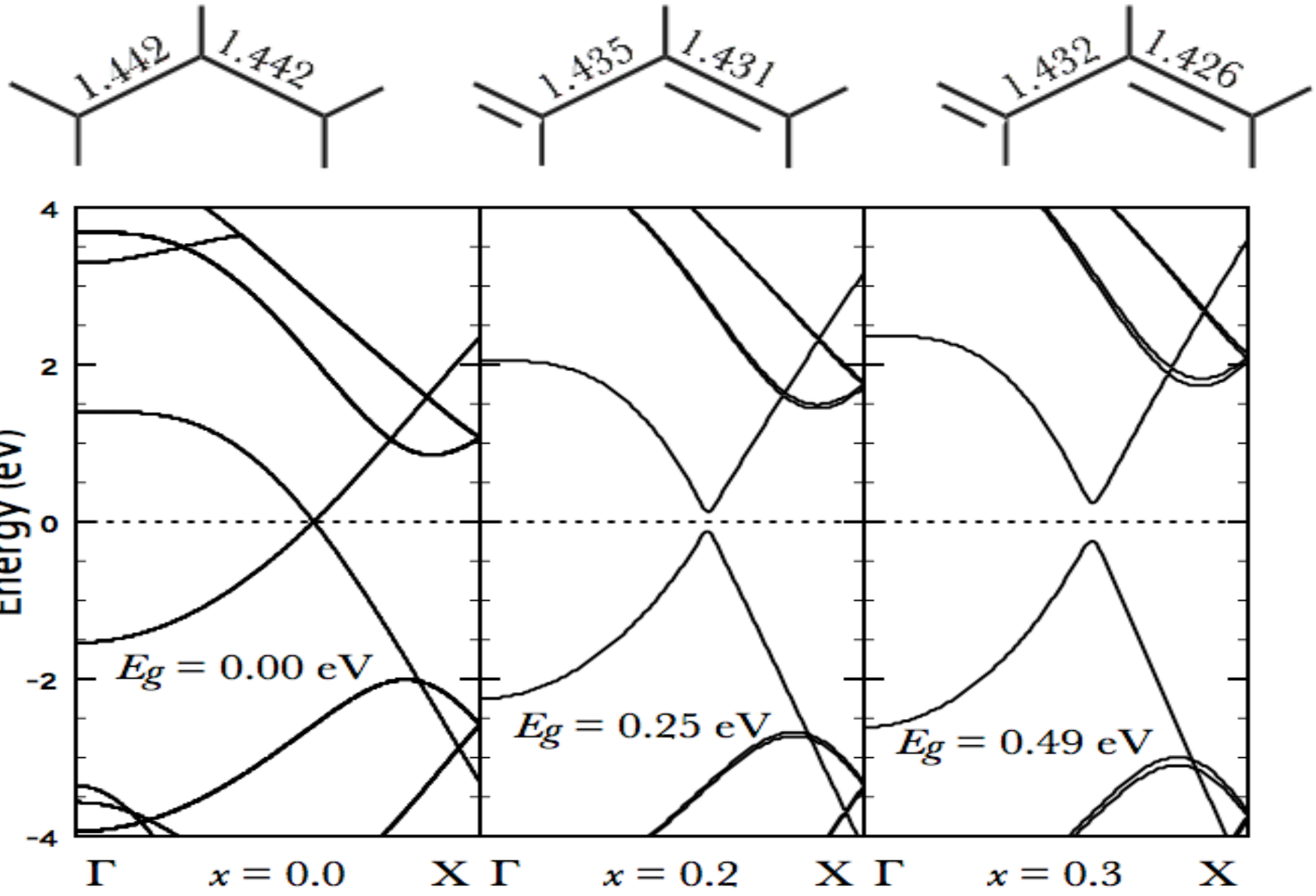
The band gap is also proportional to *x*

	Values of bond lengths and band gap of PA			
Qty	EXP	x = 0.0	B3LYP	x = 0.3
C–C (Å)	1.44	1.41	1.43	1.43
C=C (Å)	1.36	1.40	1.47	1.36
Gap (eV)	1.50	0.16	1.25	1.81

x = 0.3 gives good agreement for the gap

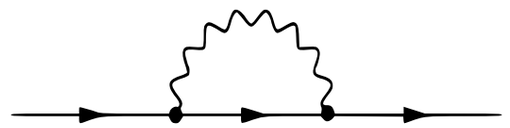
Band structure of (3,3) CNT

All bond lenghts are in Å



Since the agreement was good for the band gap of PA, we could mesure a band gap of the order of 0.5 eV in a (3,3) at low temperature.

From a density functional point a view



$$\delta n(r) = \int dr' \chi(r - r') \delta v(r') \qquad \chi(r, r') = \frac{\partial n(r)}{\partial v(r')}$$

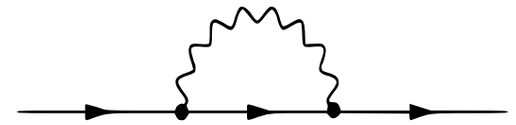
$$\delta n(r) = \int dr' \chi^s(r - r') \delta v^s(r') \qquad \chi^s(r, r') = \frac{\partial n(r)}{\partial v^s(r')}$$

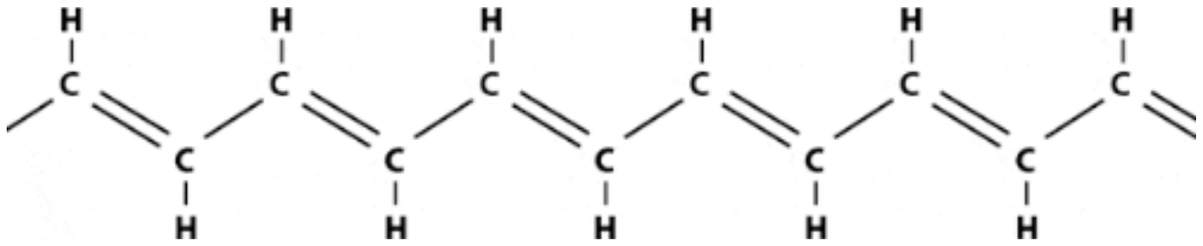
$$v^s(r) = v(r) + \int dr' \frac{n(r')}{|r - r'|} + v_{xc}(r)$$

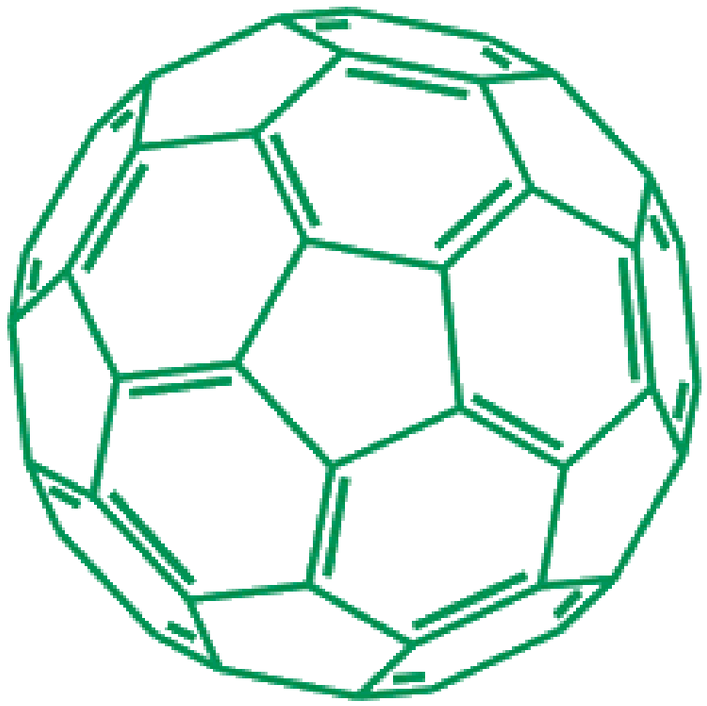
$$\frac{1}{\chi^s(r, r')} = \frac{1}{\chi(r, r')} + \frac{1}{|r - r'|} + f_{xc}(r, r')$$

$$-|\chi| = \frac{-|\chi^s|}{1 + |\chi^s| \left(\frac{1}{|r - r'|} + f_{xc} \right)}$$

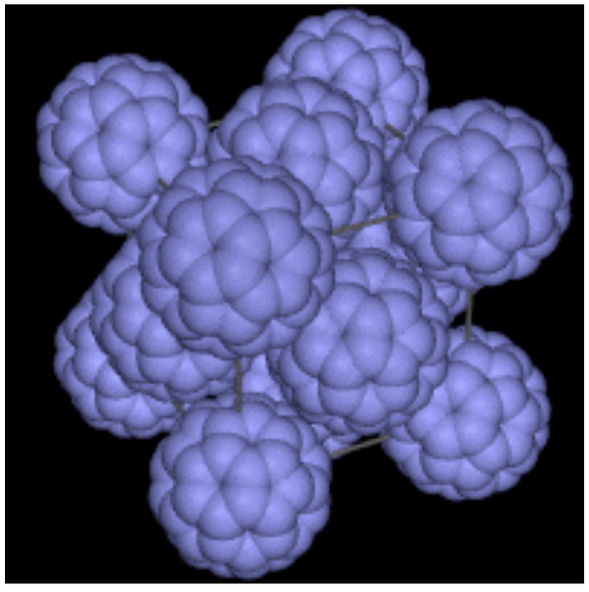
Polyacetylene and C_{60}

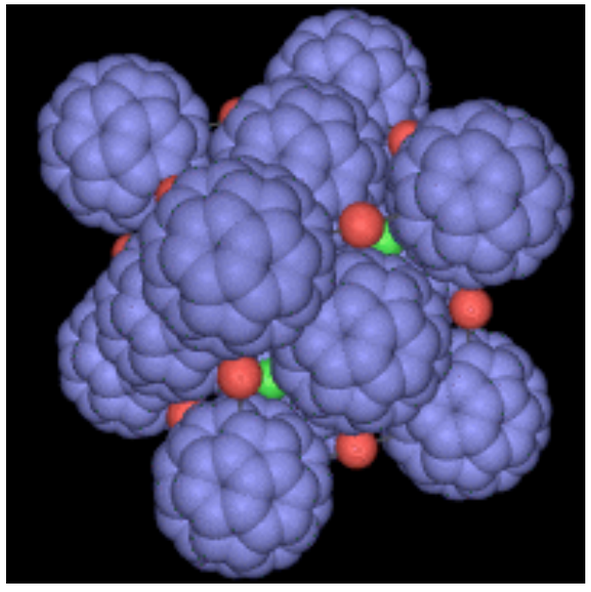




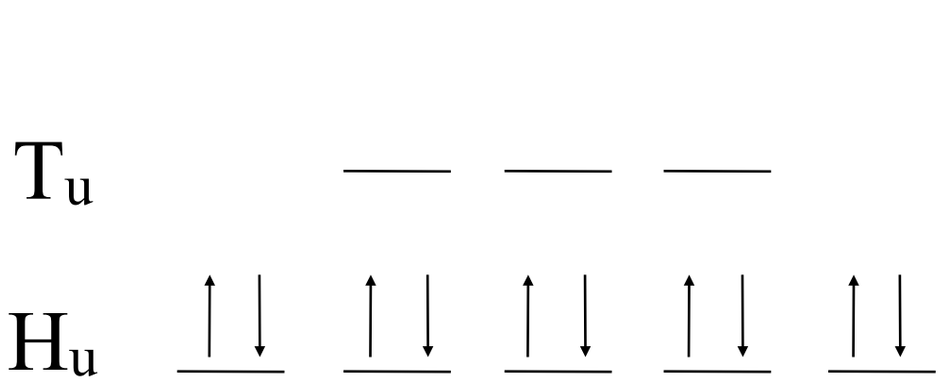


Superconductivity in C_{60} crystal





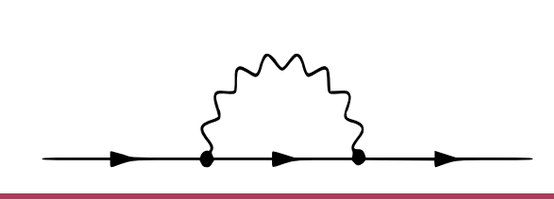
fcc fcc

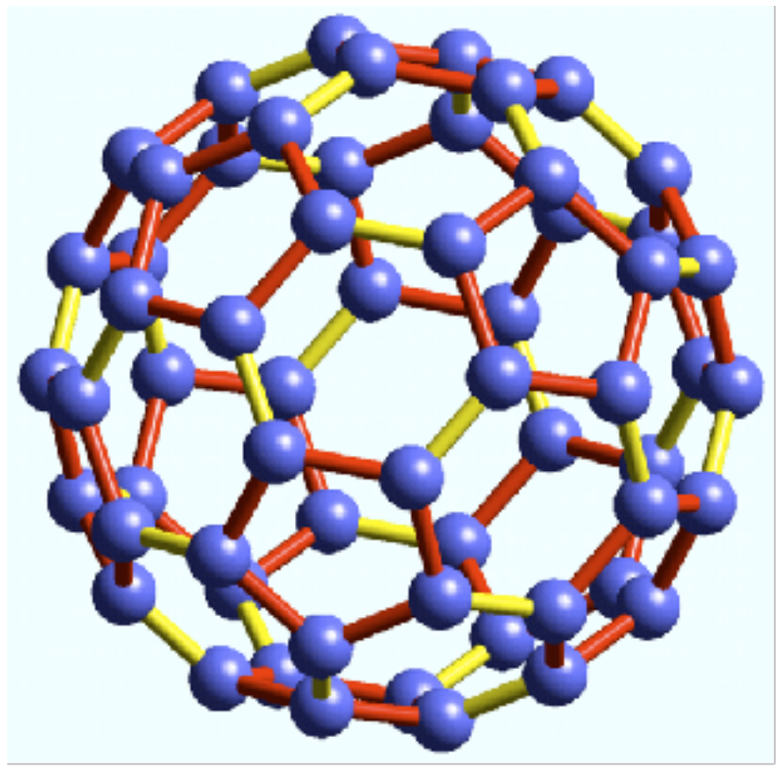


$$V_{ep} = \sum_{\alpha} \frac{1}{M\omega_{\alpha}^2} \frac{1}{g^2} \sum_{i,j=1}^{g} |\langle i|\boldsymbol{\epsilon}_{\alpha} \cdot \nabla V|j\rangle|^2$$

$$T_C \sim \theta_D \, e^{-1/V_{ep} D(\varepsilon_F)}$$

Structure

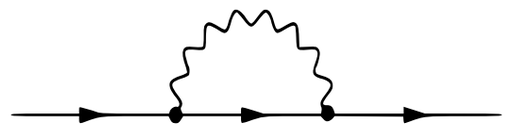




Structure

Bond (A)	Exp.	PBE	PBE 30%	B3LYP
Single	1.455	1.457 (0.1%)	1.446 (-0.6%)	1.453 (-0.1%)
Double	1.391	1.405 (1.0%)	1.389 (-0.2%)	1.395 (0.3%)

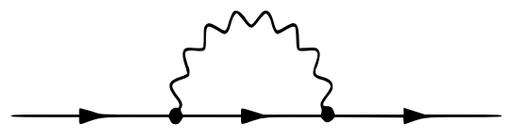
Phonon frequencies



Phonons frequencies

Mode	Frequency (cm^{-1})							
	Exp.	PBE		PBE 30%		B3LYP	
Ag1	496	488	(-2%)	505	(2%)	497	(0%)
Ag2	1470	1485	(1%)	1560	(6%)	1503	(2%)
Hg1	273	256	(-6%)	256	(-6%)	265	(-3%)
Hg2	437	415	(-5%)	406	(-7%)	433	(-1%)
Hg3	710	683	(-4%)	679	(-4%)	715	(1%)
Hg4	774	771	(-0%)	793	(2%)	786	(2%)
Hg5	1099	1101	(0%)	1130	(3%)	1126	(2%)
Hg6	1250	1256	(0%)	1299	(4%)	1276	(2%)
Hg7	1428	1435	(1%)	1503	(5%)	1454	(2%)
Hg8	1575	1570	(-0%)	1631	(4%)	1617	(3%)
Δ max			(-6%)		(-7%)		(-3%)

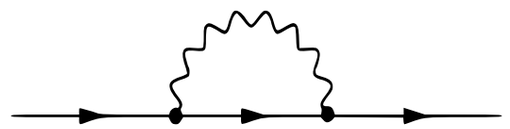
Electron-phonon coupling



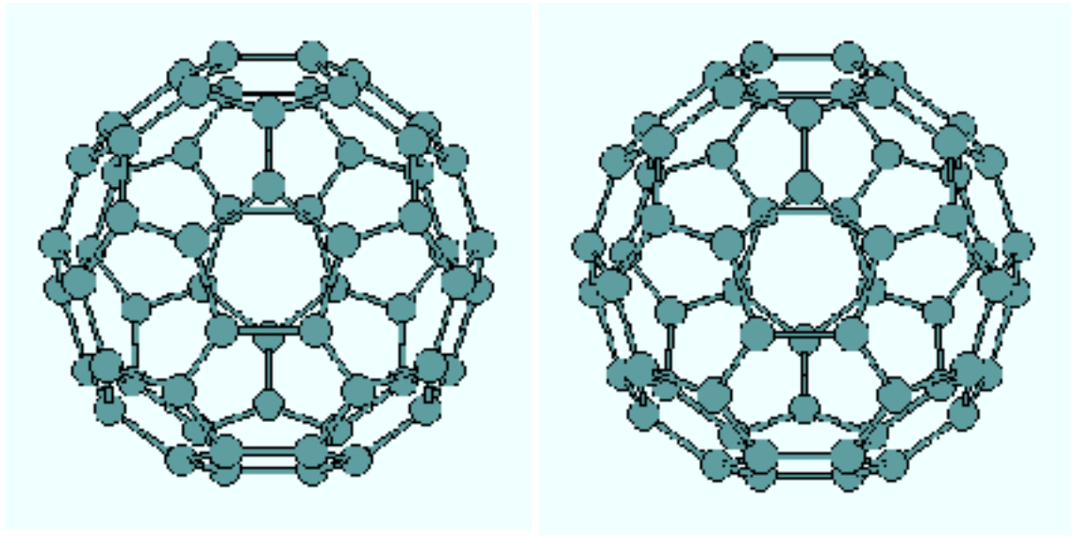
electron-phonon coupling

Mode	V_{ep} (meV)				
	PBE	PBE 30%		B3LYP	
Ag1	1.2	1.2	(0%)	1.2	
Ag2	7.4	11.8	(60%)	10.6	
Hg1	4.7	5.1	(8%)	5.8	
Hg2	11.6	14.1	(22%)	11.5	
Hg3	10.4	16.3	(57%)	12.3	
Hg4	3.7	3.8	(3%)	4.7	
Hg5	4.1	5.6	(37%)	4.8	
Hg6	2.3	3.6	(54%)	2.0	
Hg7	13.7	20.3	(49%)	20.0	
Hg8	12.2	16.2	(33%)	14.0	
Total Ag	8.6	13.1	(52%)	11.8	
Total Hg	62.6	85.0	(36%)	75.1	
Total	71.3	98.1	(38%)	87.0	(22%)

Electron-phonon coupling

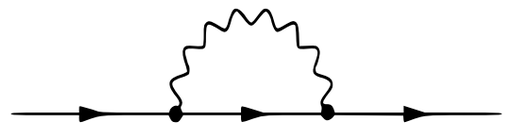


	Ag1	Ag2
PBE	1.2	7.4
PBE 30%	1.2 (0%)	11.8 (60%)



- Change in functional affects the way charge reorganize
  - Ag1 show uniform bond stretching: don’t allow for charge reorganisation =>functional shouldn’t have a strong impact
  - Ag2 show uneven bond stretching: allow for charge reorganisation =>functional could have a strong impact

Is LDA good enough?



PHYSICAL REVIEW B **84**, 155104 (2011)

Electron-phonon coupling in the C_{60} fullerene within the many-body *GW* approach

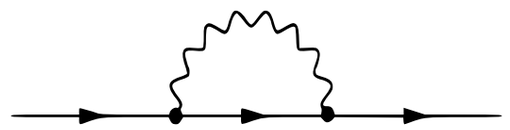
Carina Faber,[1,2] Jonathan Laflamme Janssen,[3] Michel Côté,[3] E. Runge,[2] and X. Blase[1]

LDA underestimate electron-phonon coupling.

$$\lambda = V_{\mathrm{ep}} \cdot DOS(e_F)$$

	LDA	GW	Exp.
Vep (meV)	73.4	108.6	106.8-158.3

Other example where LDA is not enough



PHYSICAL REVIEW B **78**, 081406(R) (2008)

Impact of the electron-electron correlation on phonon dispersion: Failure of LDA and GGA DFT functionals in graphene and graphite

Michele Lazzeri,[1] Claudio Attaccalite,[2] Ludger Wirtz,[3] and Francesco Mauri[1]

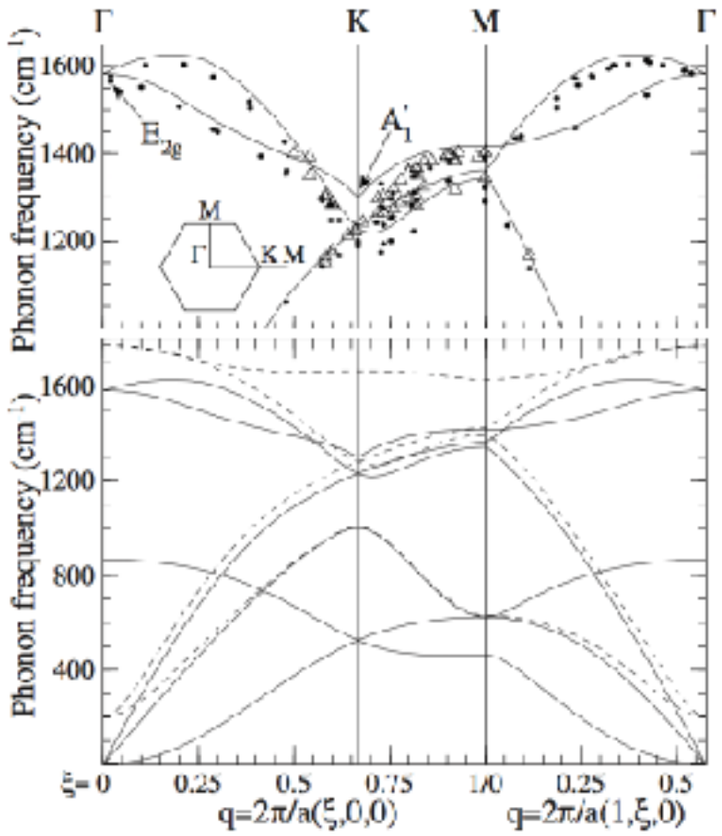
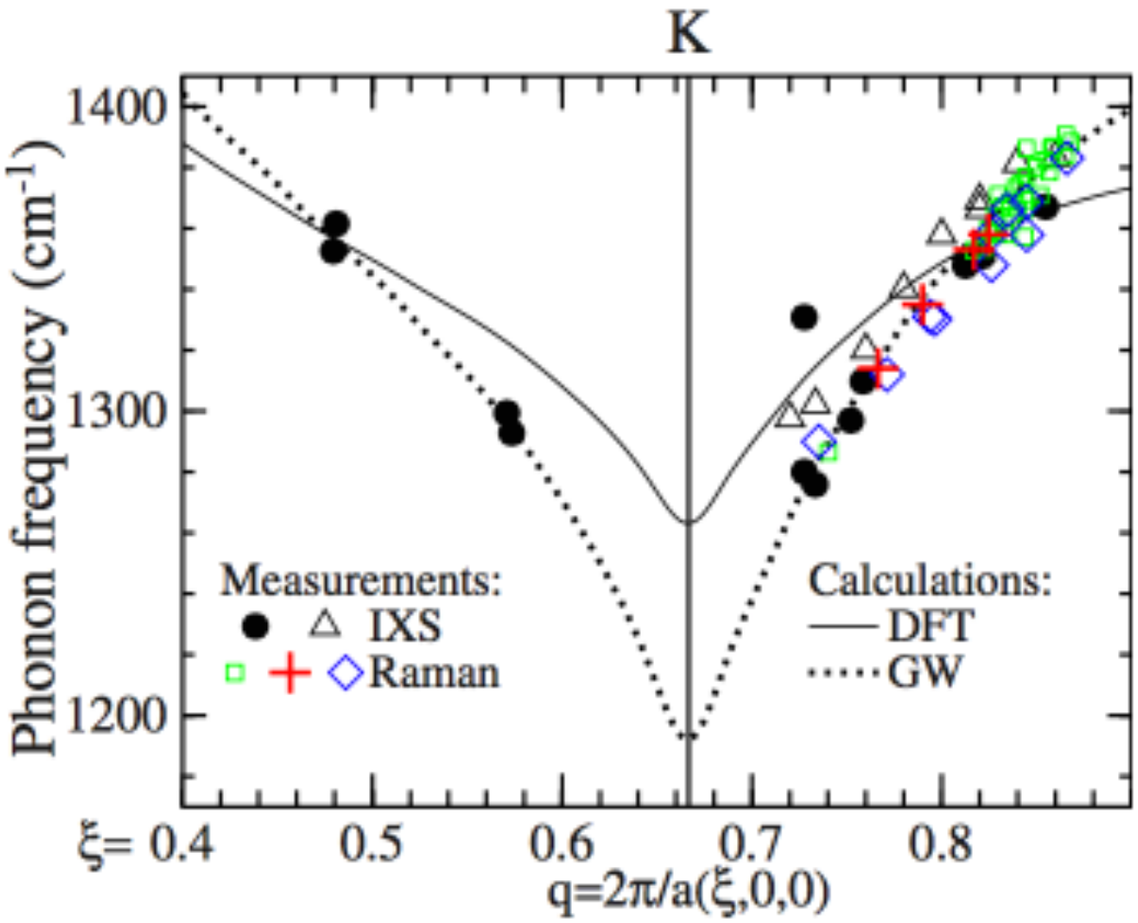
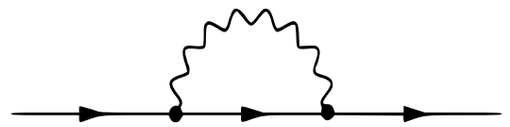


FIG. 1. Upper panel: Phonon dispersion of graphite. Lines are DFT calculations, dots and triangles are IXS measurements from Refs. 8 and 9, respectively. Lower panel: Phonon dispersion of graphene from DFT calculations. Dashed lines are obtained by subtracting, from the dynamical matrix, the phonon self-energy between the π bands ($\tilde{\omega}_q$ in the text).



another example



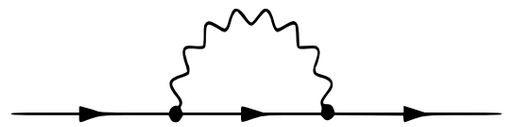
PHYSICAL REVIEW X 3, 021011 (2013)

Correlation-Enhanced Electron-Phonon Coupling: Applications of *GW* and Screened Hybrid Functional to Bismuthates, Chloronitrides, and Other High-T_c Superconductors

Z. P. Yin,* A. Kutepov, and G. Kotliar

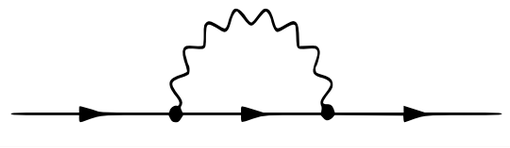
Compounds	Mode	D (LDA)	D (HSE)	λ(LDA)	λ (HSE)	$\omega_{\log}$ (LDA)	$\omega_{\log}$(HSE)	T_c(LDA)	T_c (HSE)	T_c (experiment)
$BaBiO_3$	O breathing at R	7.6	13.3	0.33	1.0	550	450	0.6	31	32.0 [1]
$BaPbO_3$	O breathing at R	10.1	11.2	0.58	0.72	500	480	10.3	18	···
$Ba_3Bi_2O_7$	O breathing at R	Approximately 0	Approximately 0	Approximately 0	Approximately 0	···	···	Approximately 0	Approximately 0	<2 [72]
ZrNCl	E_g at Γ (in plane)	2.9–4.0	3.9–4.7	0.52	0.8	422	390	6.0	18	16 [73]
HfNCl	E_g at Γ (in plane)	3.8–4.4	5.1–5.3		1.1	340	310	···	25	25.5 [2]

Outline



- Introduction/Motivations
- Theory: Allen-Heine-Cardona
- Calculations for diamond
  - at the density-functional theory level
  - at the GW method level
  - including anharmonic effects
  - including dynamical effects
- Conclusion

Green's function: Hedin's equations



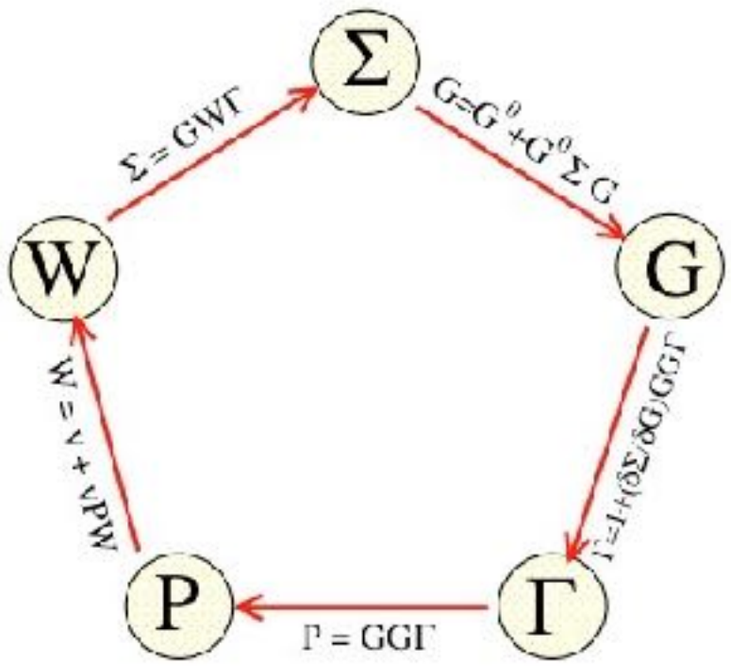
$$G(1,2) = G_0(1,2) + \int G_0(1,3)\Sigma(3,4)G(4,2)d(3,4)$$

$$\Sigma(1,2) = i\int G(1,3)\Gamma(3,2,4)W(4,1^+)d(3,4)$$

$$W(1,2) = v(1,2) + \int v(1,3)P(3,4)W(4,2)d(3,4)$$

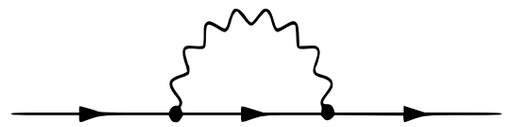
$$P(1,2) = -i\int G(1,3)\Gamma(3,4,2)G(4,1^+)d(3,4)$$

$$\Gamma(1,2,3) = \delta(1,2)\delta(1,3) + \int \frac{\partial\Sigma(1,2)}{\partial G(4,5)}G(4,6)\Gamma(6,7,3)G(7,5)d(4,5,6,7)$$



$$G^{(0)}(\mathbf{r},\mathbf{r}',\omega) = \sum_{n\mathbf{k}} \frac{\varphi_{n\mathbf{k}}^{\mathrm{DFT}}(\mathbf{r})\varphi_{n\mathbf{k}}^{\mathrm{DFT}*}(\mathbf{r}')}{\omega - \varepsilon_{n\mathbf{k}}^{\mathrm{DFT}} + i\delta\,\mathrm{sgn}(\varepsilon_{n\mathbf{k}}^{\mathrm{DFT}} - \mu)}$$

Quasiparticle energies



In the **quasiparticle (QP) formalism**, the energies and wavefunctions are obtained by the **Dyson equation**:

$$\left(-\frac{\nabla^2}{2}+V_{ext}(\mathbf{r})+V_H(\mathbf{r})\right)\varphi_{n\mathbf{k}}(\mathbf{r})+\int d\mathbf{r}'\,\Sigma\left(\mathbf{r},\mathbf{r}',\omega=\varepsilon_{n\mathbf{k}}^{\mathrm{QP}}\right)\varphi_{n\mathbf{k}}(\mathbf{r}')=\varepsilon_{n\mathbf{k}}^{\mathrm{QP}}\varphi_{n\mathbf{k}}(\mathbf{r})$$ QP equation

which is very similar to the Kohn-Sham equation:

$$\left(-\frac{\nabla^2}{2}+V_{ext}(\mathbf{r})+V_H(\mathbf{r})\right)\varphi_{n\mathbf{k}}(\mathbf{r})+V_{xc}(\mathbf{r})\varphi_{n\mathbf{k}}(\mathbf{r})=\varepsilon_{n\mathbf{k}}^{\mathrm{DFT}}\varphi_{n\mathbf{k}}(\mathbf{r})$$ KS equation

with V_{xc} that replaces Σ, the **self-energy** (a non-local and energy dependent operator).
We can calculate the **QP (GW) corrections** to the DFT KS eigenvalues by 1st order PT:

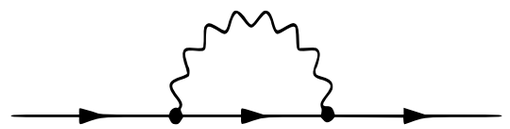
$$\varepsilon_{n\mathbf{k}}^{\mathrm{QP}}=\varepsilon_{n\mathbf{k}}^{\mathrm{DFT}}+\left\langle\varphi_{n\mathbf{k}}^{\mathrm{DFT}}\left|\Sigma(\mathbf{r},\mathbf{r}',\omega)-V_{xc}(\mathbf{r})\right|\varphi_{n\mathbf{k}}^{\mathrm{DFT}}\right\rangle$$

0-order wavefunctions

0-order

Quasiparticle correction

The GW approximation



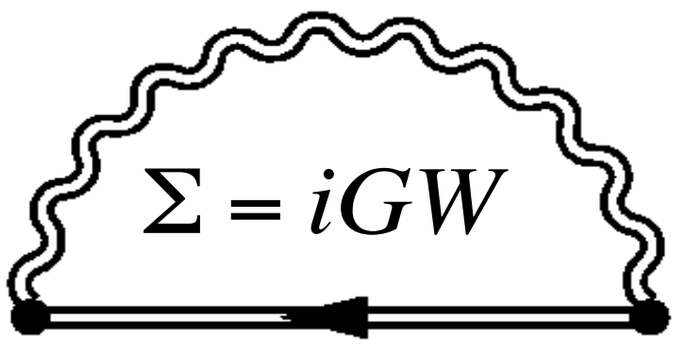
Hedin's equations:

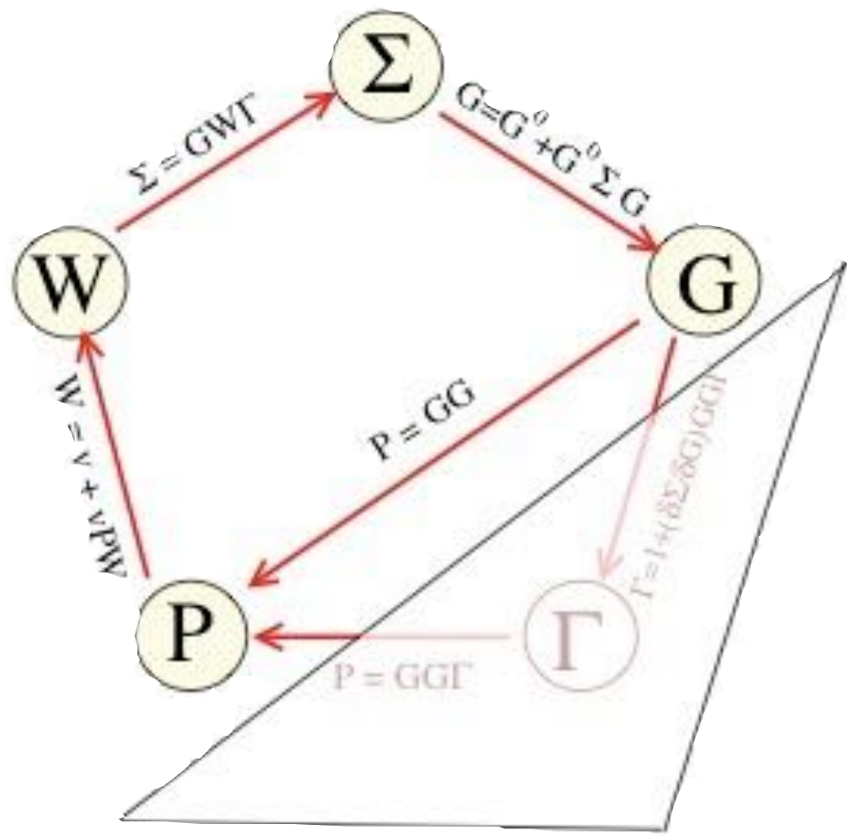
$$\Gamma(1,2,3) = \delta(1,2)\delta(1,3) \qquad \leftarrow \text{approximation to the vortex}$$

$$P(1,2) = -iG(1,2)G(2,1^+)$$

$$W(1,2) = v(1,2) - i\int v(1,3)G(3,4)G(4,3^+)W(4,2)d(3,4)$$

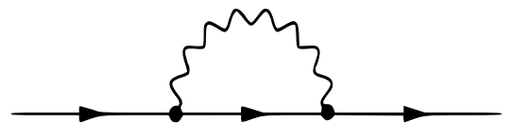
$$\Sigma(1,2) = iG(1,2)W(2,1^+)$$

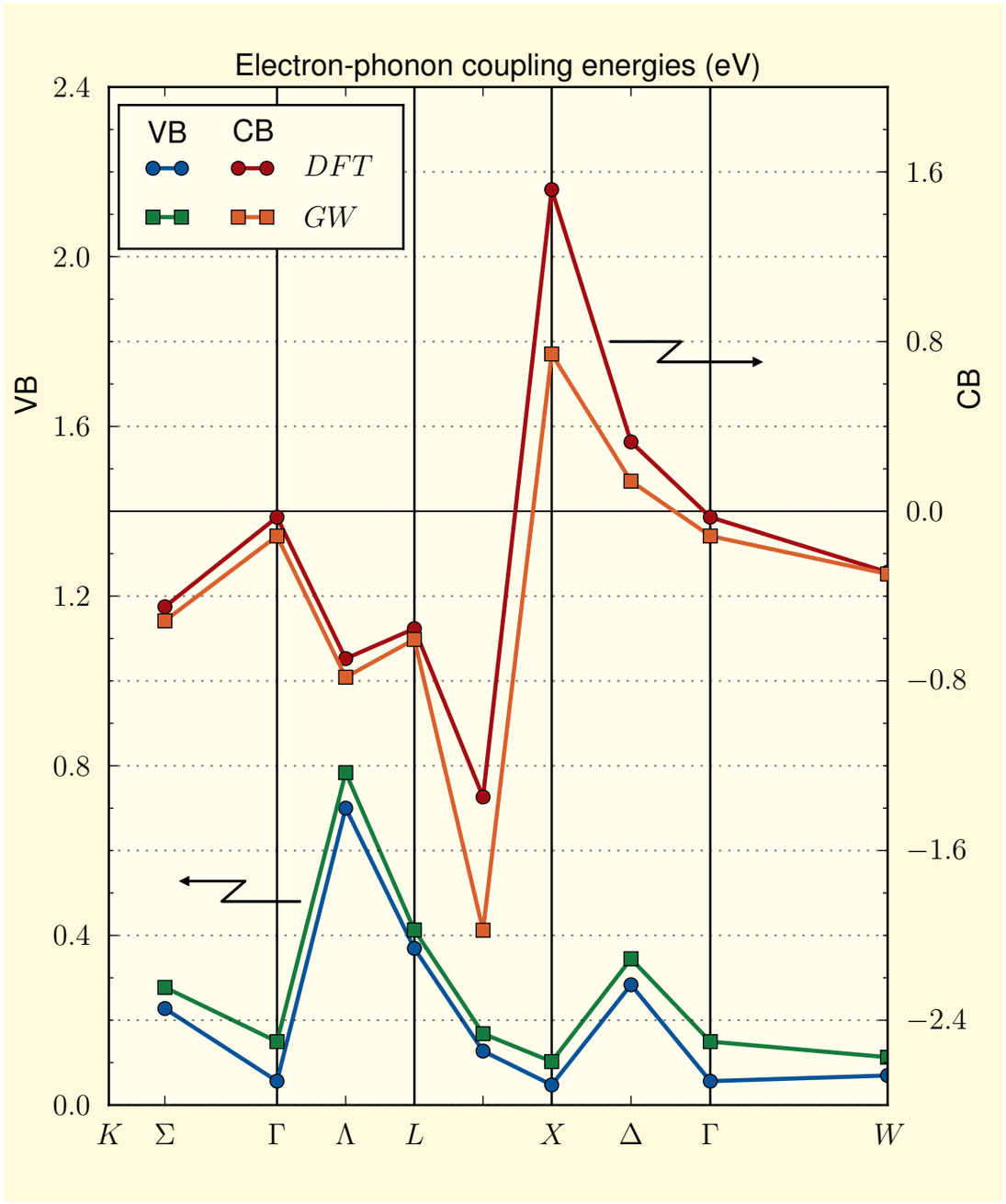




It is the RPA for the inhomogeous electron gas.

GW values : Frozen-Phonon (FP)



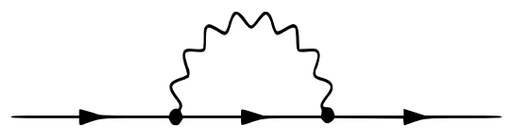


ZPR (meV)

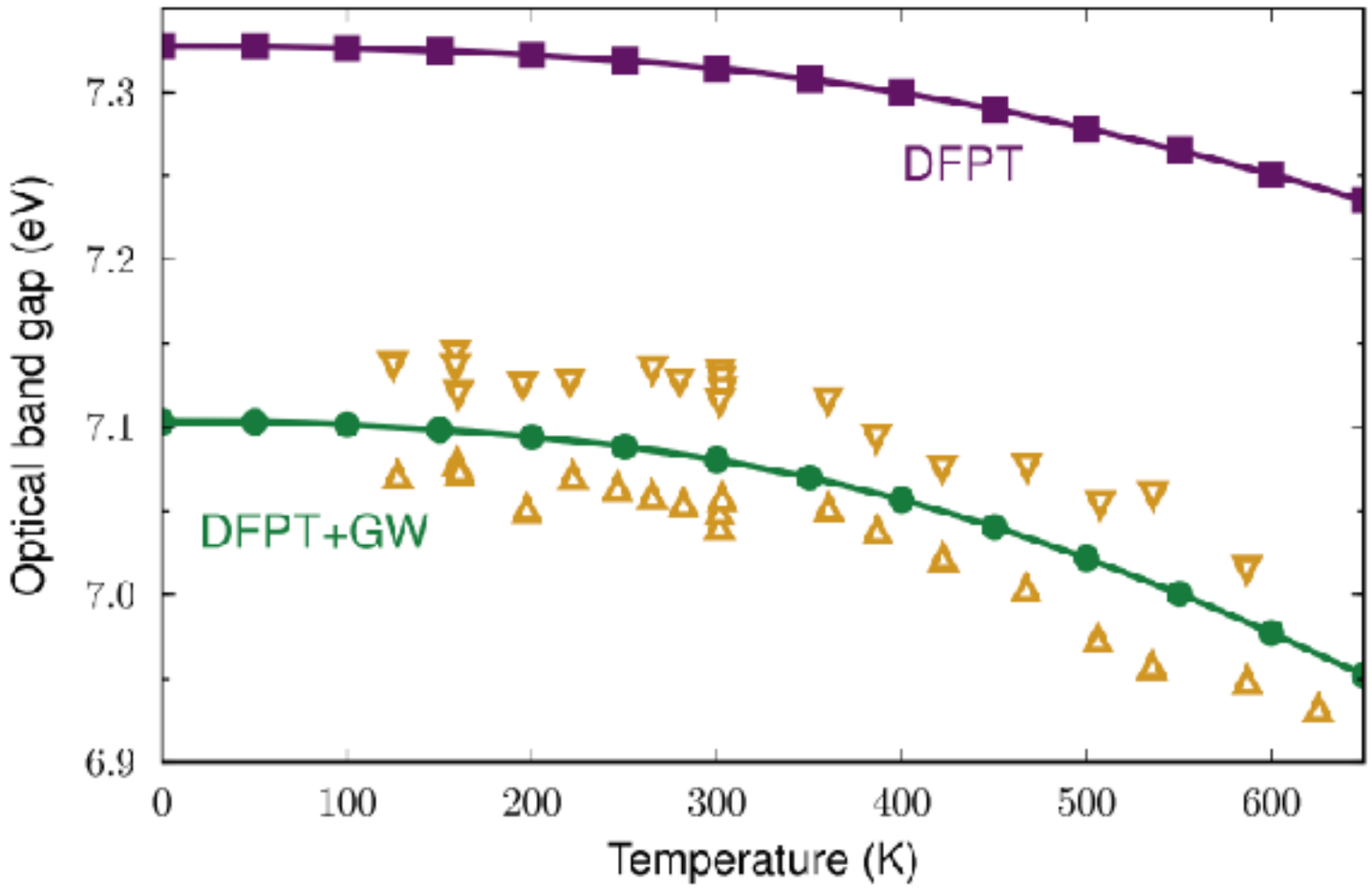
	VB	CB	Gap
FP DFT	119	-318	-437
FP *GW*	145	-477	-622
Exp.			~-600

Excellent agreement with experiment!

Temperature dependance

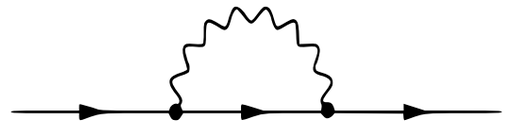


Eg(DFT) = 5.6 eV, Eg(GW) = 7.73 eV
7.73 + ZPR(DFT) = 7.3 eV
7.73 +ZPR(GW) = 7.1 eV



Slope: LDA=-0.42 meV/K, GW=-0.67 meV/K
exp: -0.60 and -0.69 meV/K

Previous works



PRL **105,** 265501 (2010) PHYSICAL REVIEW LETTERS week ending 31 DECEMBER 2010

Electron-Phonon Renormalization of the Direct Band Gap of Diamond

Feliciano Giustino,[1,2] Steven G. Louie,[2] and Marvin L. Cohen[2]

[1]*Department of Materials, University of Oxford, Parks Road, Oxford OX1 3PH, United Kingdom*
[2]*Department of Physics, University of California at Berkeley, Berkeley, California 94720, USA, and Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA*

(Received 7 September 2010; revised manuscript received 15 November 2010; published 20 December 2010)

PRL **107,** 255501 (2011) PHYSICAL REVIEW LETTERS week ending 16 DECEMBER 2011

Effect of the Quantum Zero-Point Atomic Motion on the Optical and Electronic Properties of Diamond and Trans-Polyacetylene

Elena Cannuccia[1] and Andrea Marini[2]

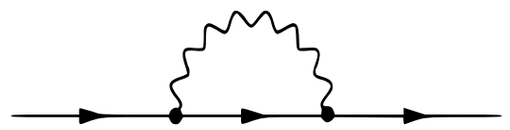
PHYSICAL REVIEW B VOLUME 27, NUMBER 8 15 APRIL 1983

Temperature dependence of the direct gap of Si and Ge

P. B. Allen
Department of Physics, State University of New York at Stony Brook, Stony Brook, New York 11794

M. Cardona
Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-7000 Stuttgart 80, Federal Republic of Germany

(Received 18 October 1982)

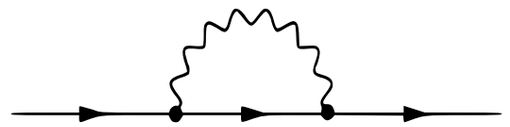


Many-Body Effects on the Zero-Point Renormalization of the Band Structure

G. Antonius,[1,*] S. Poncé,[2] P. Boulanger,[3] M. Côté,[1] and X. Gonze[2]
[1]*Département de physique, Université de Montréal, C.P. 6128, Succursale Centre-Ville, Montréal, Canada H3C 3J7*
[2]*IMCN-NAPS, Université catholique de Louvain, Place Croix du Sud 1, B-1348 Louvain-la-Neuve, Belgium*
[3]*Institut Néel, 25 avenue des Martyrs, BP 166, 38042 Grenoble cedex 9, France*
(Received 31 May 2013; revised manuscript received 16 May 2014; published 29 May 2014)

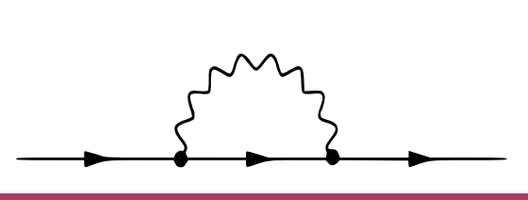
doi: 10.1103/PhysRevLett.112.215501

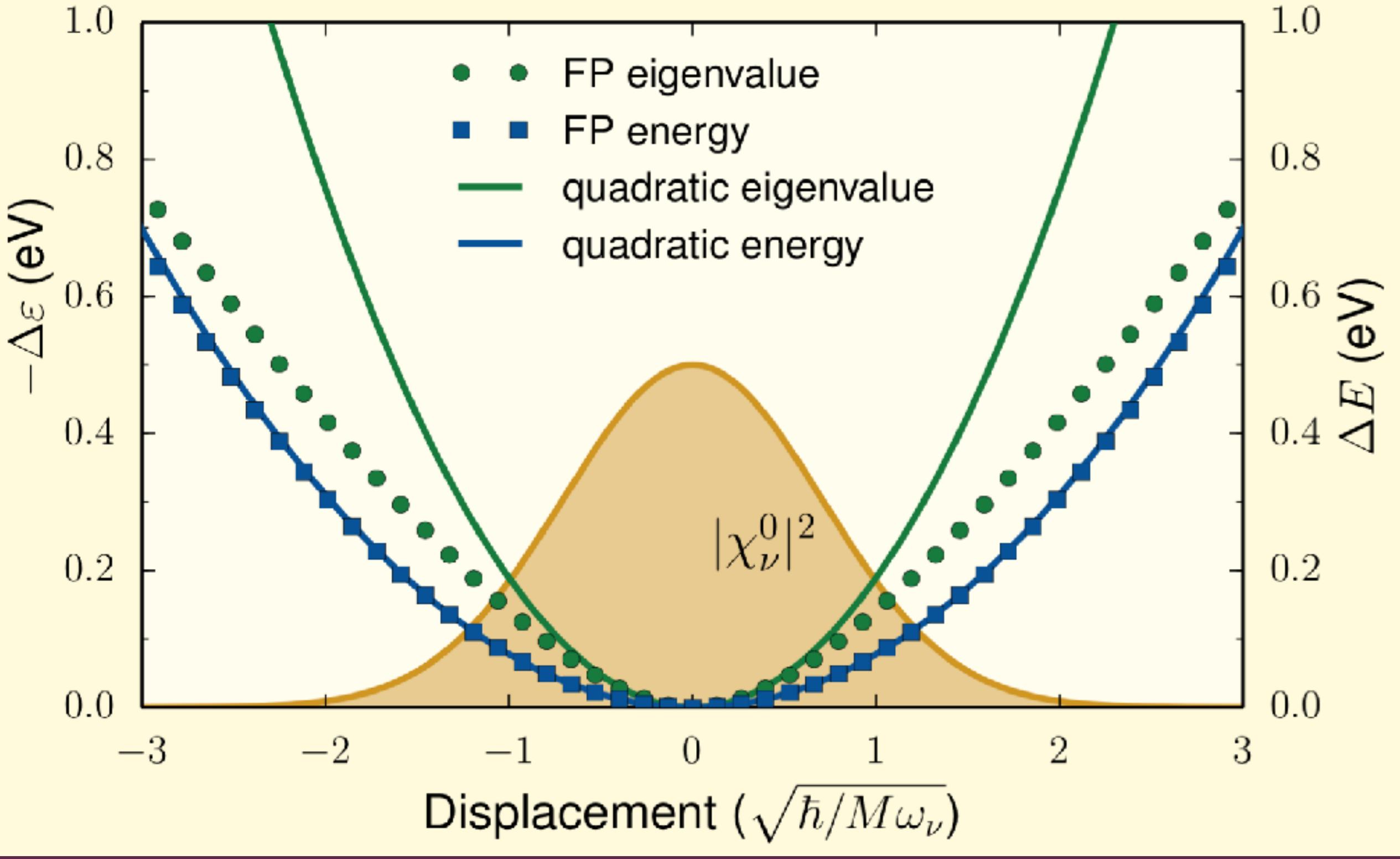
Outline



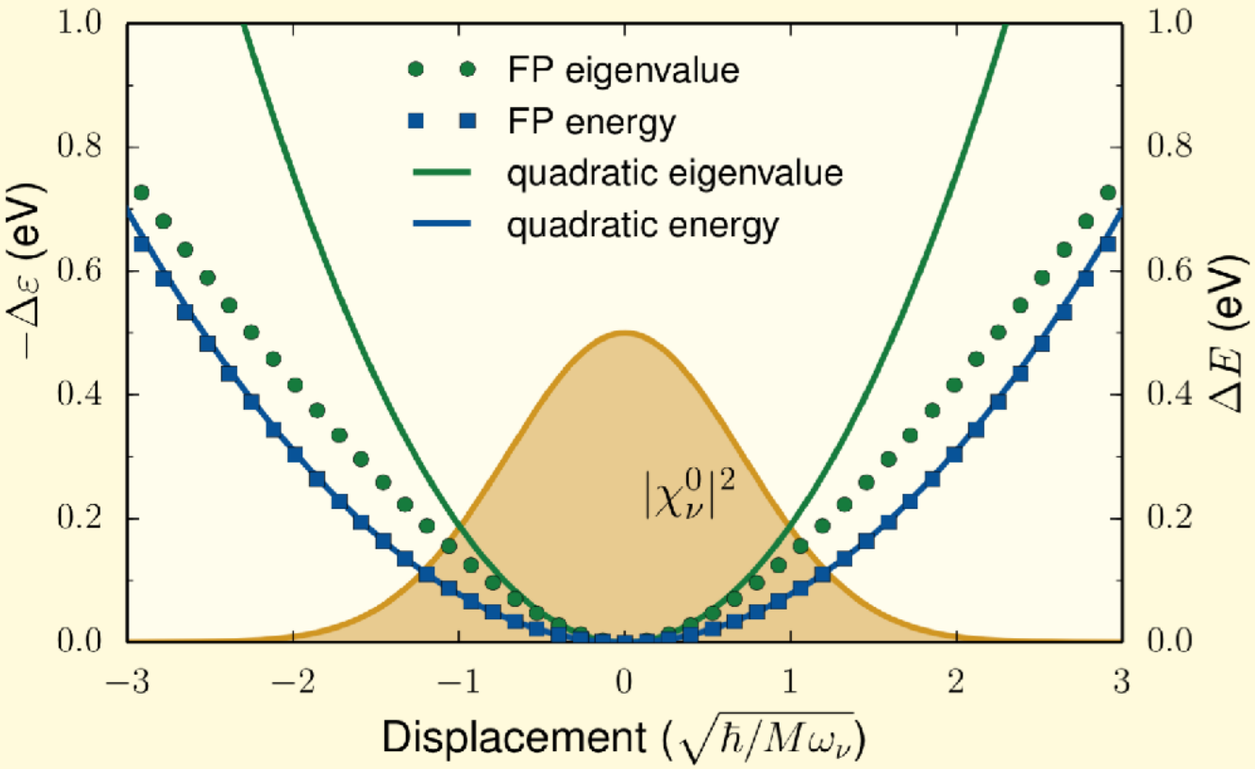
- Introduction/Motivations
- Theory: Allen-Heine-Carbona
- Calculations for diamond
  - at the density-functional theory level
  - at the GW method level
  - including anharmonic effects
  - including dynamical effects
- Conclusion

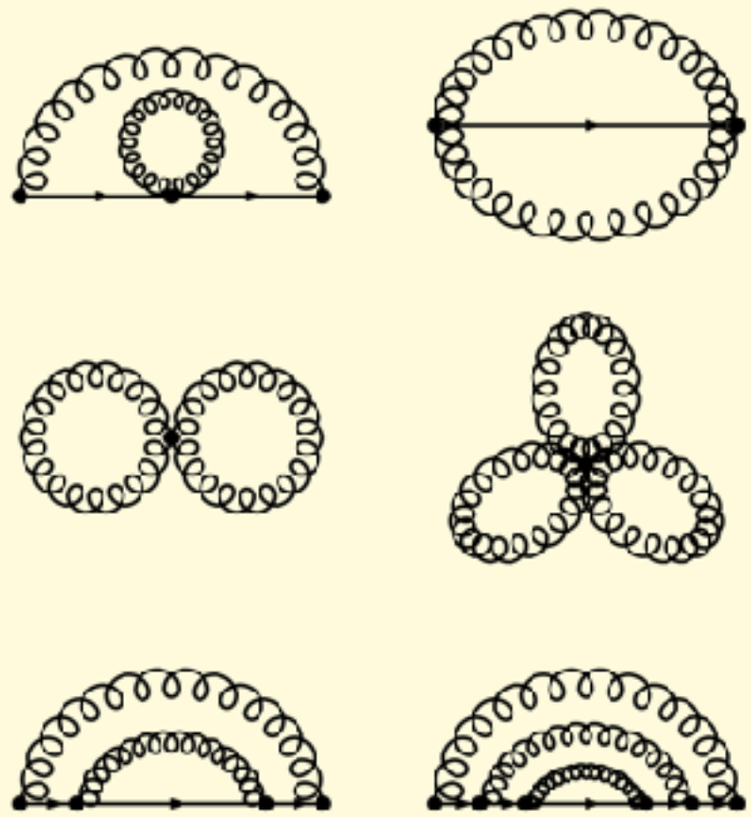
Anharmonic effects





Anharmonic effects

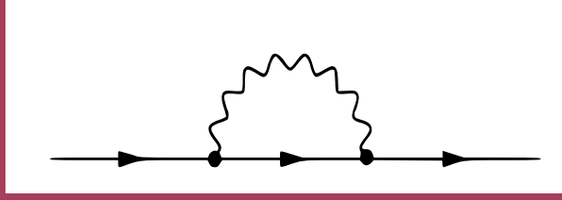


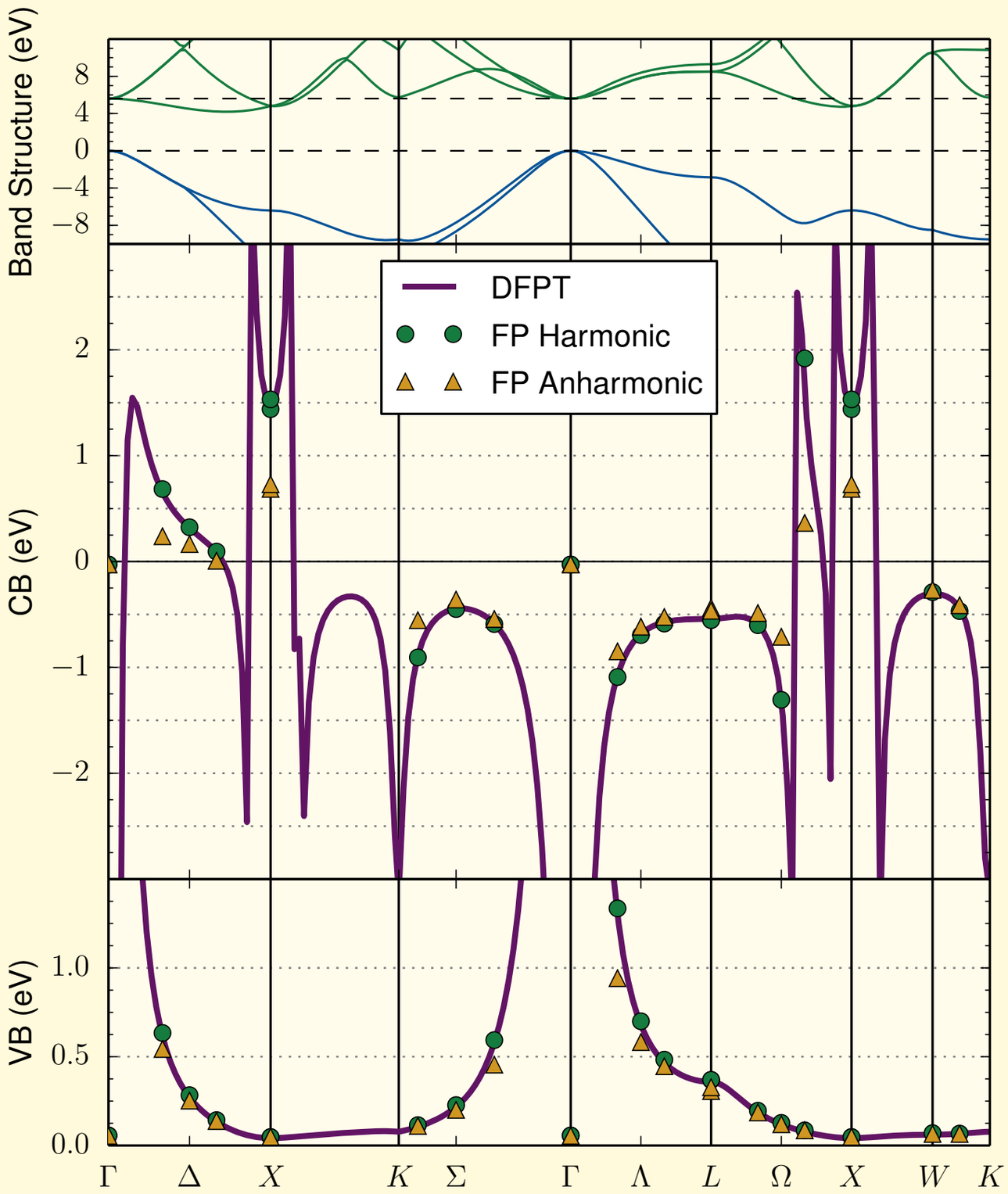


Non-perturbative expression for the renormalized eigenvalue:

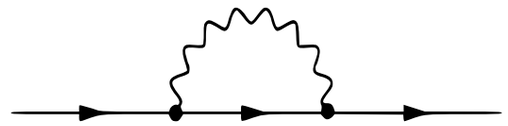
$$\varepsilon_i = \sum_\nu \int |\chi_\nu(z)|^2 \, \varepsilon_i\left[z\ \mathbf{u}^\nu_\kappa\right] dz$$

Anharmonic effect

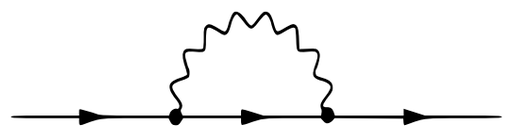




Results



	VB	CB	Gap
FP DFT	119	-318	-437
FP *GW*	145	-477	-622
FP Anh.(DFT)	104	-208	-312
GW+Anh(app.)	145	-390	-535
Exp.			~-600

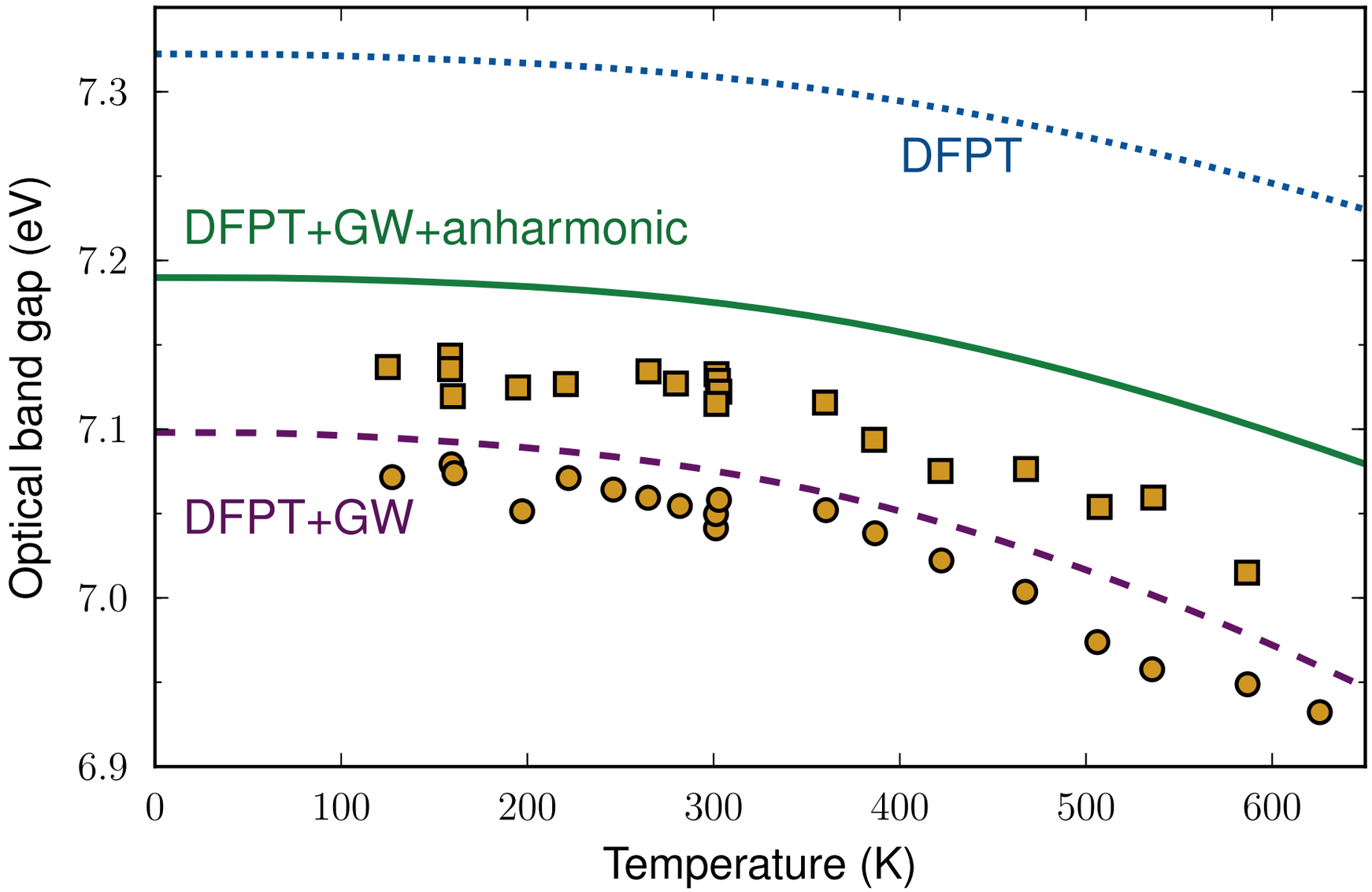


Eg(DFT) = 5.6 eV, Eg(GW) = 7.73 eV

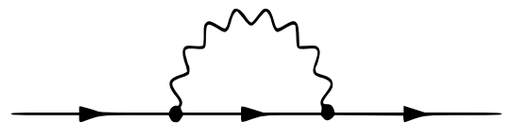
7.73 + ZPR(DFT) = 7.3 eV

7.73 +ZPR(GW) = 7.1 eV

7.73+ZPR(GW+Anh.) = 7.2 eV



Dynamical effects in ZPR



PHYSICAL REVIEW B **92**, 085137 (2015)

Dynamical and anharmonic effects on the electron-phonon coupling and the zero-point renormalization of the electronic structure

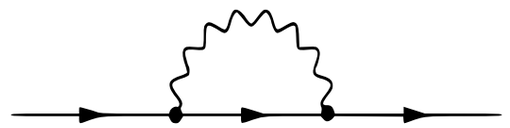
G. Antonius,[1,*] S. Poncé,[2] E. Lantagne-Hurtubise,[1] G. Auclair,[1] X. Gonze,[2] and M. Côté[1]
[1]*Département de physique, Université de Montréal, C.P. 6128, Succursale Centre-Ville, Montréal, Canada H3C 3J7*
[2]*Institute of Condensed Matter and Nanosciences, Université catholique de Louvain, B-1348 Louvain-la-Neuve, Belgium*

$$\Sigma^{ep}_{\lambda\lambda'}(\omega) = \Sigma^{Fan}_{\lambda\lambda'}(\omega) + \Sigma^{DW}_{\lambda\lambda'}$$

$$\Sigma^{Fan}_{\lambda\lambda'}(\omega) = \sum_{\nu} \frac{1}{2\omega_\nu} \sum_{\lambda''} \langle\psi_\lambda| V^{(1)}_\nu |\psi_{\lambda''}\rangle \langle\psi_{\lambda''}| V^{(1)*}_\nu |\psi_{\lambda'}\rangle \left[\frac{n_\nu(T) + f_{\lambda''}(T)}{\omega - \varepsilon^0_{\lambda''} + \omega_\nu + i\eta\ \mathrm{sgn}(\omega)} + \frac{n_\nu(T) + 1 - f_{\lambda''}(T)}{\omega - \varepsilon^0_{\lambda''} - \omega_\nu + i\eta\ \mathrm{sgn}(\omega)} \right]$$

$$\Sigma^{DW}_{\lambda\lambda'} = \sum_{\nu} \frac{1}{2\omega_\nu} \langle\psi_\lambda| V^{(2)}_{\nu\nu} |\psi_{\lambda'}\rangle \left[2n_\nu(T) + 1\right]$$

Practical calculations



Now we can calculate the Green function:

$$G_\lambda(\omega) \approx \left(\omega - \varepsilon^0_\lambda - \Sigma^{ep}_\lambda(\omega)\right)^{-1}$$

Experimentally we observe ARPES which is related to the spectral function:

$$A_\lambda(\omega) = \frac{1}{\pi} \frac{|\mathfrak{Im}\Sigma^{ep}_\lambda(\omega)|}{[\omega - \varepsilon^0_\lambda - \mathfrak{Re}\Sigma^{ep}_\lambda(\omega)]^2 + \mathfrak{Im}\Sigma^{ep}_\lambda(\omega)^2}$$

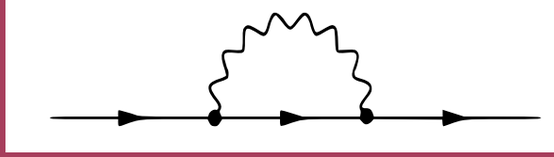
The energy correction can be evaluated by the peak in the spectral function:

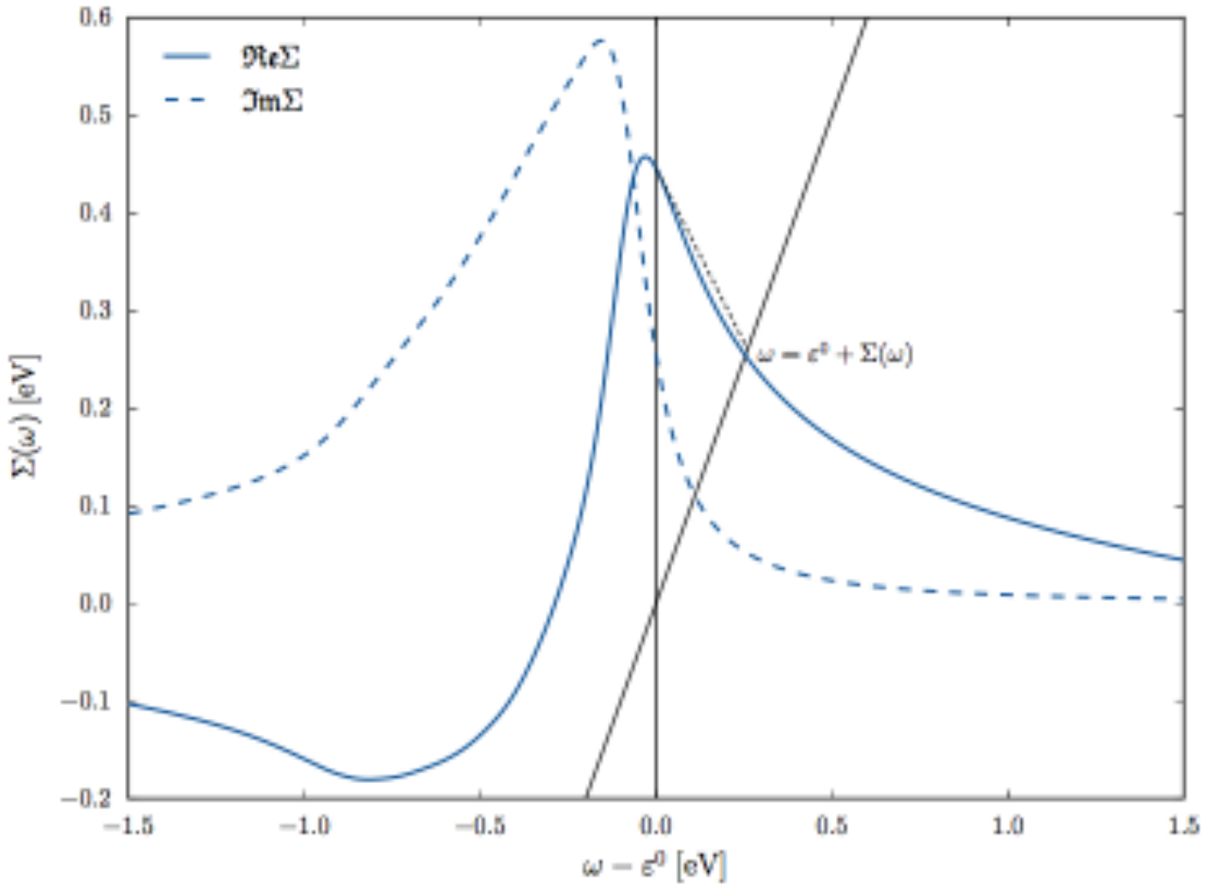
$$\varepsilon_\lambda = \varepsilon^0_\lambda + \mathfrak{Re}\Sigma^{ep}_\lambda(\varepsilon_\lambda)$$

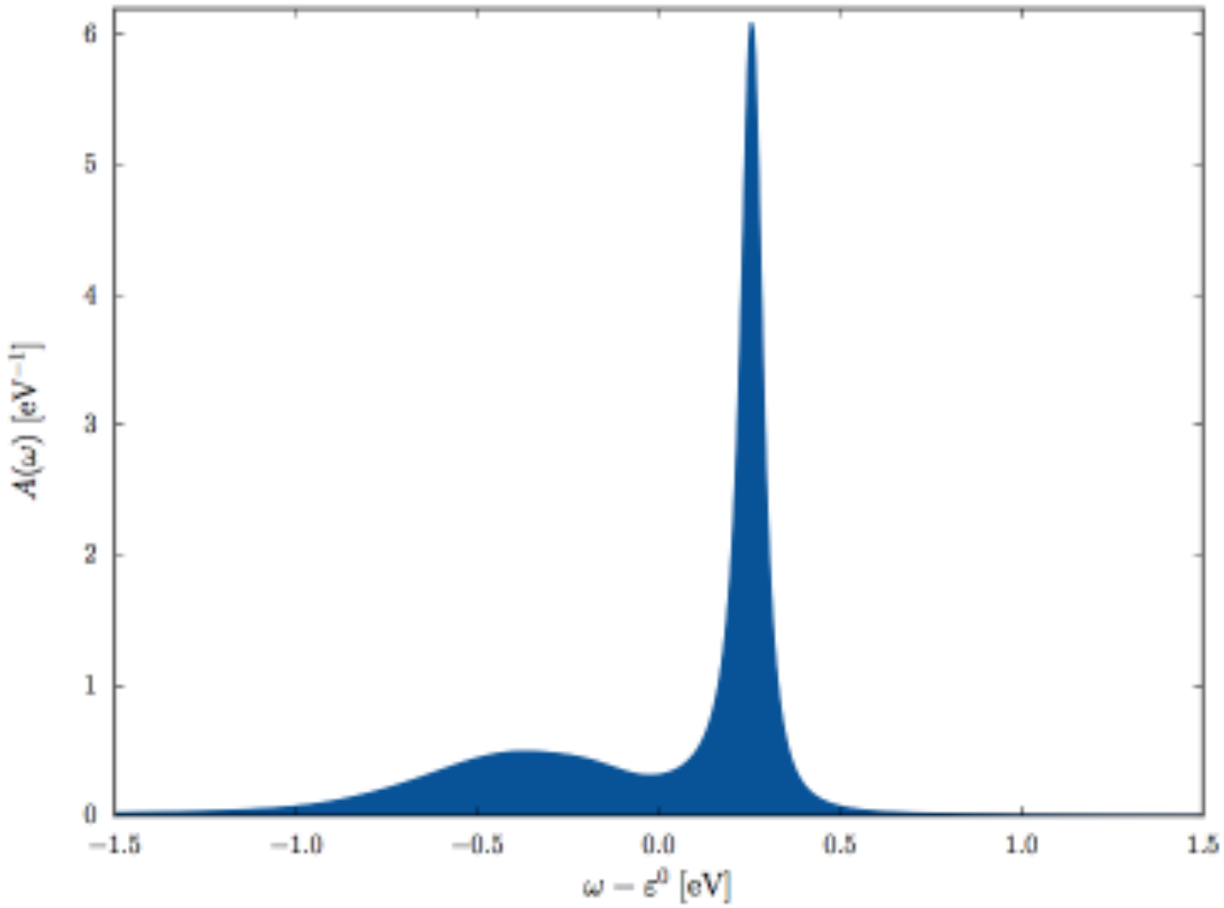
Often, the following approximation is made:

$$\varepsilon_\lambda \approx \varepsilon^0_\lambda + Z_\lambda \mathfrak{Re}\Sigma^{ep}_\lambda(\varepsilon^0_\lambda) \qquad Z_\lambda = \left(1 - \mathfrak{Re}\frac{\partial \Sigma^{ep}_\lambda(\omega)}{\partial \omega}\Big|_{\omega=\varepsilon^0_\lambda}\right)^{-1}$$

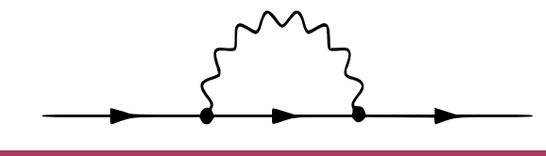
The case of valence band of LiF

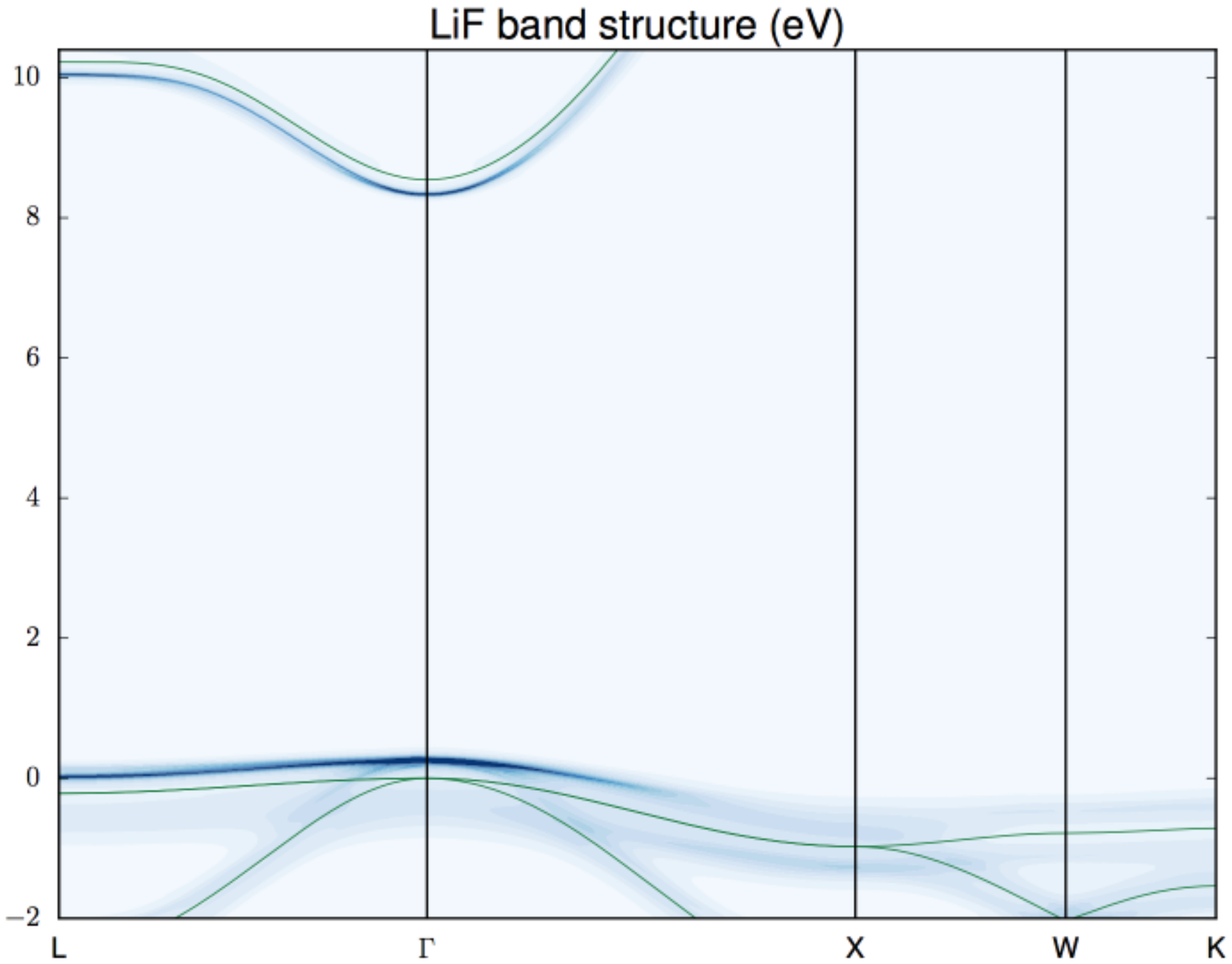




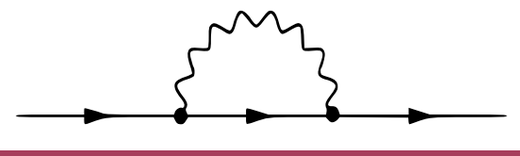


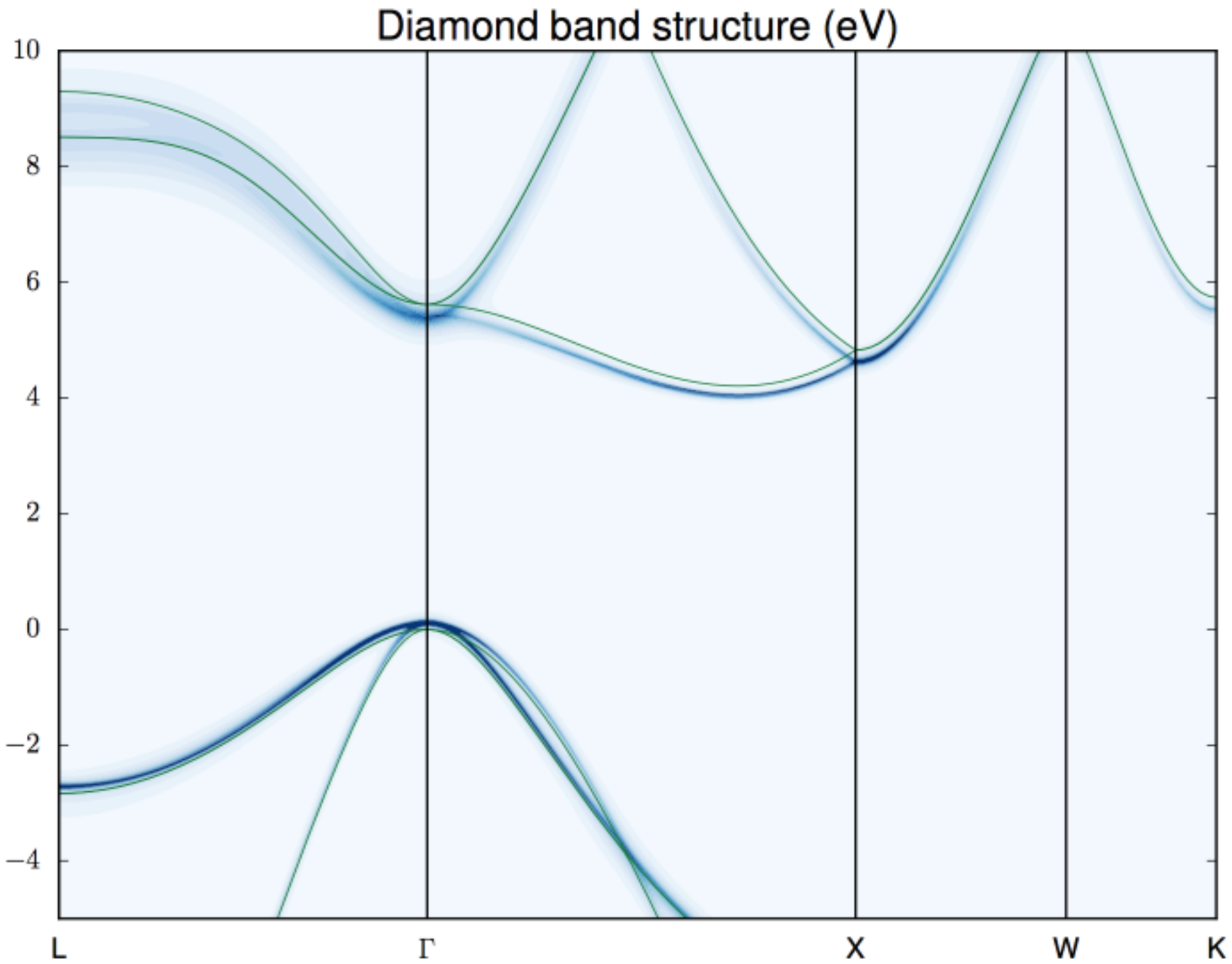
Band Structure of LiF



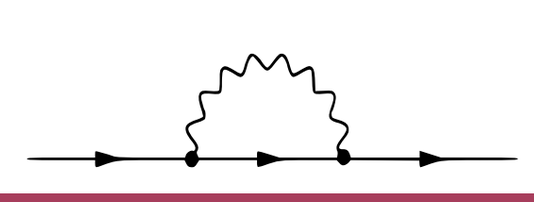


Band Structure of diamond

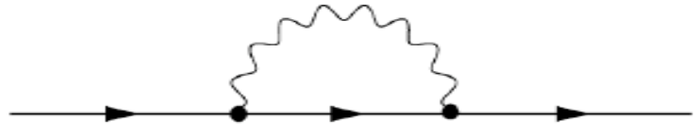




Cumulant expansion



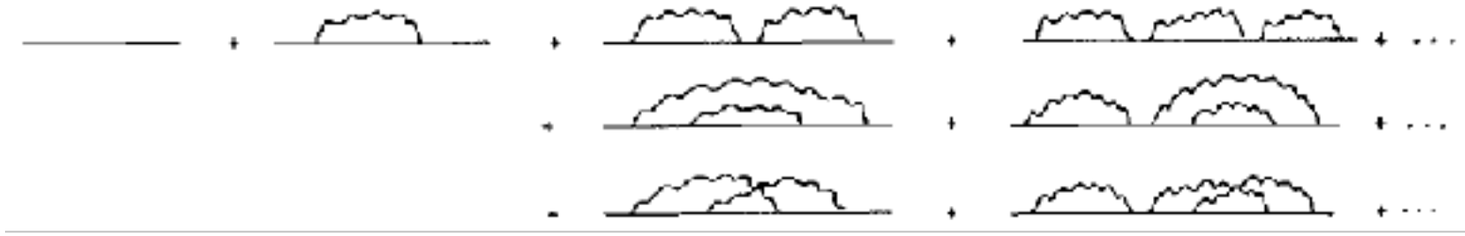
Start from Migdal self-energy



Spectral function from retarded cumulant approach

$$G_C(\mathbf{k}n,t) = G_0(\mathbf{k}n,t)e^{C(\mathbf{k}n,t)}$$

J.J. Kas, J.J. Rehr and L. Reining,
Phys. Rev. B 90, 085112 (2014)



$$\beta^R(\mathbf{k}n,\omega) = \frac{1}{\pi}|\Im m\,\Sigma^{Fan}(\mathbf{k}n,\omega+\varepsilon_{\mathbf{k}n})|$$

$$C^R(\mathbf{k}n,t) = \int_{-\infty}^{\infty}\beta^R(\mathbf{k}n,\omega)\frac{e^{-i\omega t}+i\omega t-1}{\omega^2}d\omega$$

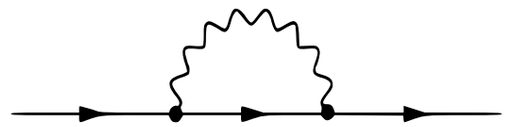
$$G_C^R(\mathbf{k}n,t) = -i\theta(t)e^{-i(\varepsilon_{\mathbf{k}n}+\Sigma^{DW}_{\mathbf{k}n})t}e^{C^R(\mathbf{k}n,t)}$$

$$G_C^R(\mathbf{k}n,\omega) = \int_{-\infty}^{\infty}e^{i\omega t}G_C^R(\mathbf{k}n,t)dt$$

Non-Dyson diagrams treated approximately

Known to give more than one satellite !

Application of cumulant expansion



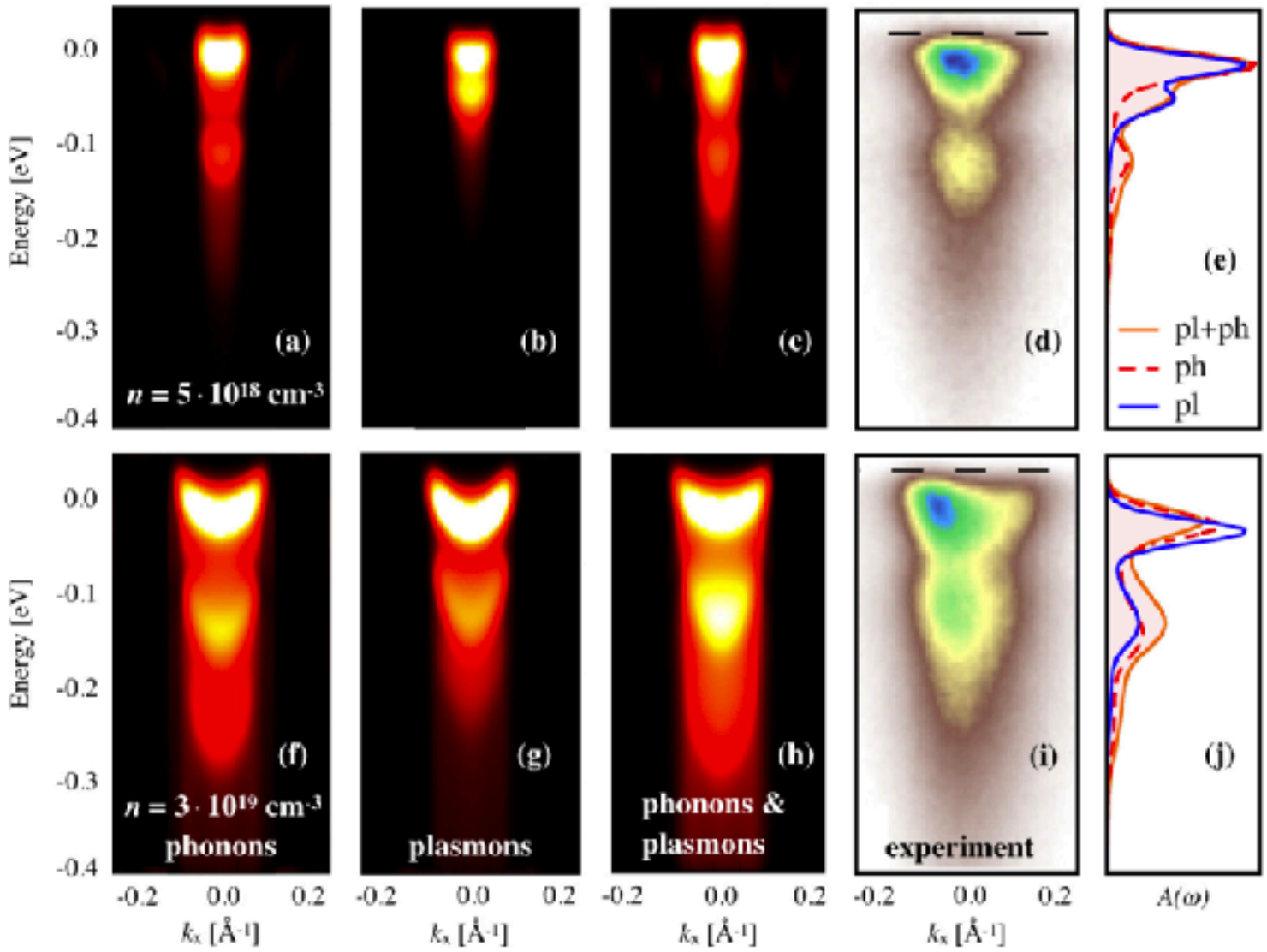
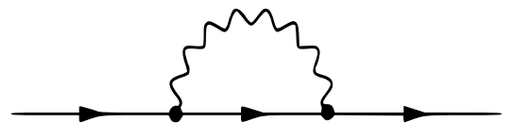


FIG. 4. (a)–(d) Spectral function of TiO_2 obtained from the cumulant expansion approach by accounting for the effects of electronic coupling to (a) phonons, (b) plasmons, and (c) both at a doping concentration of 5×10^{18} cm^{-3}. (d) Angle-resolved photoemission spectrum of TiO_2, adapted from Ref. [20]. (e) Spectral function at Γ due to plasmons (pl), phonons (ph), and their combined effect (pl+ph) from the cumulant expansion. (f)–(j) Same as above for $n = 3 \times 10^{19}$ cm^{-3}.

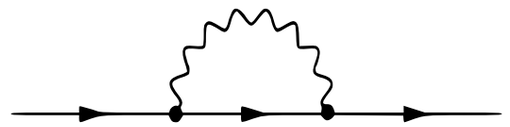
Caruso, F., Verdi, C., Poncé, S. & Giustino, F. Electron-plasmon and electron-phonon satellites in the angle-resolved photoelectron spectra of n -doped anatase TiO 2. *Physical Review B* **97,** 165113 (2018).

Outline



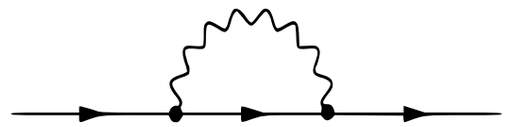
- Introduction/Motivations
- Theory: Allen-Heine-Cardona
- Calculations for diamond
  - at the density-functional theory level
  - at the GW method level
  - including anharmonic effects
  - including dynamical effects
- Conclusion

Conclusion



- Renormalization of the Eg due to ZPR can be large for light atoms crystals.
- Self-energy of the eigenvalues by the phonon coupling is necessary to obtain precise values.
- Can be readily computed with DFT, but careful to the choice of the functional.
- Green's function approach (GW) gives results in better agreement with experiment, but implementation is limited.
- Anharmonic effects can be large and need to pay attention to dynamical effects for certain systems.

References

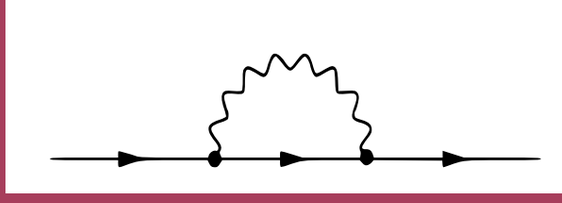


References :

• X. Gonze, P. Boulanger and M. Côté, *Ann. Phys* 523, 168 (2011*)*
• S. Poncé *et al, Comput. Materials Science* 83, 341 (2014*)*
• G. Antonius, S. Poncé, P. Boulanger, M. Côté and X. Gonze, *Phys. Rev. Lett.*112, 215501 (2014)
• S. Poncé *et al, Phys. Rev. B*. 90, 214304 (2014)
• S. Poncé *et al, J. Phys. Chem* 143, 102813 (2015)
• G. Antonius *et al, Phys. Rev. B* 92, 085137 (2015)
• J.-P. Néry, P.B. Allen, G. Antonius, L. Reining, A. Miglio, and X. Gonze *Phys. Rev. B* 97, 115145 (2018*)*

Also :

• *Many-body perturbation theory approach to the electron-phonon interaction with density-functional theory as a starting point,* A. Marini, S. Poncé and X. Gonze, *Phys. Rev. B* 91, 224310 (2015)
• *Electron-phonon interactions from first principles*, F. Giustino, *Rev. Mod. Phys.* 89**,** 015003 (2017)



Lesson TDepES

Temperature-DEPendence of the Electronic Structure.

This lesson aims at showing how to get the following physical properties, for periodic solids:

- The zero-point-motion renormalization (ZPR) of eigenenergies
- The temperature-dependence of eigenenergies
- The lifetime/broadening of eigenenergies

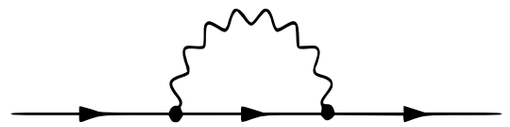
It should take about 1 hour.

For the theory related to the temperature-dependent calculations, please read the following papers: *[Ponce2015]*, *[Ponce2014]* and *[Ponce2014a]*.

There are two ways to compute the temperature dependence with Abinit:

- **Using Anaddb**: historically the first implementation. This option does not require Netcdf.
- **Using post-processing python scripts**: this is the recommended approach as it provides more options and is more efficient (less disk space, less memory demanding). This option **requires Netcdf** (both in Abinit and python). In this tutorial, we only focus on the netCDF-based approach.

Acknowledgment



Financial

CRSNG NSERC

Fonds de recherche Nature et technologies Québec

Computational ressources

compute • calcul CANADA

Calcul Québec

Thank you!