density-functional perturbation theory

response functions, phonons, and all that

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response functions

$$\text{property} = \frac{\partial(\text{variable})}{\partial(\text{strength})}$$

response functions

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- ☛ polarizability, dielectric constant $\qquad \dfrac{\partial \mathsf{P}_i}{\partial \mathsf{E}_j}$
- ☛ elastic constants $\qquad \dfrac{\partial \sigma_{ij}}{\partial \epsilon_{kl}}$
- ☛ piezoelectric constants $\qquad \dfrac{\partial \mathsf{P}_i}{\partial \epsilon_{kl}}$
- ☛ interatomic force constants $\qquad \dfrac{\partial f_i^s}{\partial u_j^t}$
- ☛ Born effective charges $\qquad \dfrac{\partial d_i^s}{\partial u_j^s}$
- ☛ ... $\qquad$ ...

susceptibilities as energy derivatives

$$\hat{H}_\alpha = \hat{H}^\circ + \alpha \hat{A}$$

$$\chi_{BA} = \frac{\partial \langle \hat{B} \rangle_\alpha}{\partial \alpha}$$

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$$\langle \hat{B} \rangle = \frac{\partial E_\beta}{\partial \beta}$$

(Hellmann & Feynman)

$$\hat{H}_\beta = \hat{H}^\circ + \beta \hat{B}$$

susceptibilities as energy derivatives

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(Hellmann & Feynman)

$$\hat{H}_\beta = \hat{H}^\circ + \beta \hat{B}$$

$$\boxed{\chi_{BA} = \frac{\partial^2 E_{\alpha\beta}}{\partial \alpha \partial \beta}}$$

$$\hat{H}_{\alpha\beta} = \hat{H}^\circ + \alpha \hat{A} + \beta \hat{B}$$

energy derivatives

$$H = H_0 + \sum_i \lambda_i v_i$$

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$$E[\lambda] = E_0 - \sum_i f_i \lambda_i + \frac{1}{2} \sum_{ij} h_{ij} \lambda_i \lambda_j + \cdots$$

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☛ structural optimization & molecular dynamics

energy derivatives

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- ☛ structural optimization & molecular dynamics
- ☛ (static) response functions
  - elastic constants
  - dielectric tensor
  - piezoelectric tensor
  - ...
- ☛ vibrational modes in the adiabatic approximation
  - interatomic force constants
  - Born effective charges
  - ...

energy derivatives from perturbation

$$H = H_0 + \sum_i \lambda_i v_i \qquad\qquad E[\lambda] = E_0 - \sum_i f_i \lambda_i + \frac{1}{2} \sum_{ij} h_{ij} \lambda_i \lambda_j + \cdots$$

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energy derivatives from perturbation

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$$f_i = - \left. \frac{\partial E}{\partial \lambda_i} \right|_{\lambda=0} = -\langle \Psi_0 | v_i | \Psi_0 \rangle$$

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energy derivatives from perturbation

$$H = H_0 + \sum_i \lambda_i v_i \qquad E[\lambda] = E_0 - \sum_i f_i \lambda_i + \frac{1}{2} \sum_{ij} h_{ij} \lambda_i \lambda_j + \cdots$$

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$$h_{ij} = \left. \frac{\partial^2 E}{\partial \lambda_i \partial \lambda_j} \right|_{\lambda=0} = 2 \sum_n \frac{\langle \Psi_0 | v_i | \Psi_n \rangle \langle \Psi_n | v_j | \Psi_0 \rangle}{\epsilon_0 - \epsilon_n}$$

energy derivatives from perturbation

$$H = H_0 + \sum_i \lambda_i v_i \qquad\qquad E[\lambda] = E_0 - \sum_i f_i \lambda_i + \frac{1}{2} \sum_{ij} h_{ij} \lambda_i \lambda_j + \cdots$$

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$$\begin{aligned} h_{ij} = \left. \frac{\partial^2 E}{\partial \lambda_i \partial \lambda_j} \right|_{\lambda=0} \quad &= \quad 2 \sum_n \frac{\langle \Psi_0 | v_i | \Psi_n \rangle \langle \Psi_n | v_j | \Psi_0 \rangle}{\epsilon_0 - \epsilon_n} \\ &= \quad 2 \langle \Psi_0 | v_i | \Psi'_j \rangle \end{aligned}$$

energy derivatives from perturbation

$$H = H_0 + \sum_i \lambda_i v_i \qquad\qquad E[\lambda] = E_0 - \sum_i f_i \lambda_i + \frac{1}{2}\sum_{ij} h_{ij}\lambda_i\lambda_j + \cdots$$

$$f_i = -\left.\frac{\partial E}{\partial \lambda_i}\right|_{\lambda=0} = -\langle \Psi_0 | v_i | \Psi_0 \rangle \qquad = \int v_i(\mathbf{r})\rho_0(\mathbf{r})d\mathbf{r}$$

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the “2n+1” theorem

$$\Phi = \Phi_0 + \mathcal{O}(\epsilon) \Rightarrow E = E_0 + \mathcal{O}(\epsilon^2)$$

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$$E = \frac{\langle \Phi_0 + \Phi' | (H_0 + V') | \Phi_0 + \Phi' \rangle}{\langle \Phi_0 + \Phi' | \Phi_0 + \Phi' \rangle} + \mathcal{O}(V'^4)$$

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$$\boxed{E^{(3)} = \langle \Phi' | V' | \Phi' \rangle - \langle \Phi' | \Phi' \rangle \langle \Phi_0 | V' | \Phi_0 \rangle}$$

density-functional perturbation theory

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$$E(\lambda) = \min_n \left(F[n] + \int V_\lambda(\mathbf{r}) n(\mathbf{r}) \right) \quad \int n(\mathbf{r}) d\mathbf{r} = N$$

DFT

density-functional perturbation theory

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$$\frac{\partial E(\lambda)}{\partial \lambda_i} = \int n_\lambda(\mathbf{r}) v_i(\mathbf{r}) d\mathbf{r} \qquad \text{HF}$$

density-functional perturbation theory

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$$E(\lambda) = \min_n \left(F[n] + \int V_\lambda(\mathbf{r}) n(\mathbf{r}) \right) \quad \int n(\mathbf{r}) d\mathbf{r} = N$$ DFT

$$\frac{\partial E(\lambda)}{\partial \lambda_i} = \int n_\lambda(\mathbf{r}) v_i(\mathbf{r}) d\mathbf{r}$$ HF

$$\boxed{\frac{\partial^2 E(\lambda)}{\partial \lambda_i \partial \lambda_j} = \int \frac{\partial n_\lambda(\mathbf{r})}{\partial \lambda_j} v_i(\mathbf{r}) d\mathbf{r}}$$ DFPT

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calculating the response

$$n(\mathbf{r}) = \sum_v |\phi_v(\mathbf{r})|^2$$

$$n'(\mathbf{r}) = 2\mathrm{Re}\sum_v \phi_v^{\circ *}(\mathbf{r})\phi'_v(\mathbf{r})$$

calculating the response

$$n(\mathbf{r}) = \sum_v |\phi_v(\mathbf{r})|^2$$

$$\begin{aligned} n'(\mathbf{r}) &= 2\mathrm{Re} \sum_v \phi_v^{\circ *}(\mathbf{r}) \phi_v'(\mathbf{r}) \\ &= 2\mathrm{Re} \sum_{cv} \rho_{vc}' \phi_v^{\circ *}(\mathbf{r}) \phi_c^{\circ}(\mathbf{r}) \end{aligned}$$

$$\phi_v' = \sum_c \phi_c^\circ \frac{\langle \phi_c^\circ | V' | \phi_v^\circ \rangle}{\epsilon_v^\circ - \epsilon_c^\circ}$$

calculating the response

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$$\boxed{(H^\circ - \epsilon_v^\circ)\phi'_v = -P_c V' \phi_v^\circ}$$

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DFPT: the equations

DFT

$$V_0(\mathbf{r}) \leftrightarrows n(\mathbf{r})$$

$$V_{SCF}(\mathbf{r}) = V_0(\mathbf{r}) + \int \frac{n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} d\mathbf{r}' + \mu_{xc}(\mathbf{r})$$

$$n(\mathbf{r}) = \sum_{\epsilon_v < E_F} |\phi_v(\mathbf{r})|^2$$

$$\boxed{\big(-\Delta + V_{SCF}(\mathbf{r})\big)\phi_v(\mathbf{r}) = \epsilon_v \phi_v(\mathbf{r})}$$

DFPT: the equations

DFT

DFPT

$$V_0(\mathbf{r}) \leftrightarrows n(\mathbf{r})$$

$$V'(\mathbf{r}) \leftrightarrows n'(\mathbf{r})$$

$$V_{SCF}(\mathbf{r}) = V_0(\mathbf{r}) + \int \frac{n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} d\mathbf{r}' + \mu_{xc}(\mathbf{r}) \longrightarrow V'_{SCF}(\mathbf{r}) = V'(\mathbf{r}) + \int \frac{n'(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} d\mathbf{r}' + \mu'_{xc}(\mathbf{r})$$

$$\downarrow \qquad\qquad\qquad \downarrow$$

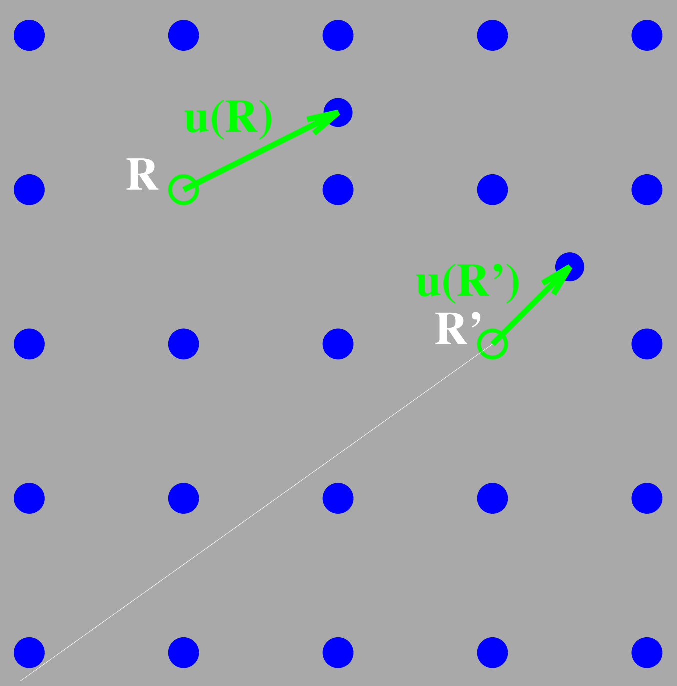
$$n(\mathbf{r}) = \sum_{\epsilon_v < E_F} |\phi_v(\mathbf{r})|^2 \longrightarrow n'(\mathbf{r}) = 2 \ \mathrm{Re} \sum_{\epsilon_v < E_F} \phi_v^*(\mathbf{r}) \phi'_v(\mathbf{r})$$

$$\downarrow \qquad\qquad\qquad \downarrow$$

$$\boxed{(-\Delta + V_{SCF}(\mathbf{r}))\phi_v(\mathbf{r}) = \epsilon_v \phi_v(\mathbf{r})} \longrightarrow \boxed{(-\Delta + V_{SCF}(\mathbf{r}) - \epsilon_v)\phi'_v(\mathbf{r}) = P_c V'_{SCF}(\mathbf{r}) \phi_v(\mathbf{r})}$$

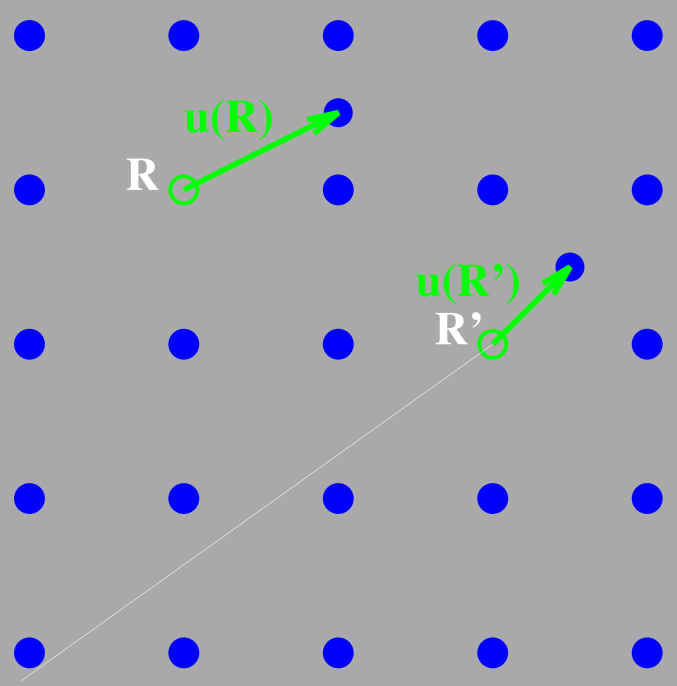
SB, P. Giannozzi, and A. Testa, Phys. Rev. Lett. **58**, 1861 (1987) simulating atomic vibrations …

lattice dynamics



$$V(\mathbf{r}) = V_0(\mathbf{r}) + \sum_{\mathbf{R}} \mathbf{u}(\mathbf{R}) \cdot \frac{\partial v(\mathbf{r}-\mathbf{R})}{\partial \mathbf{R}} + \cdots$$

lattice dynamics



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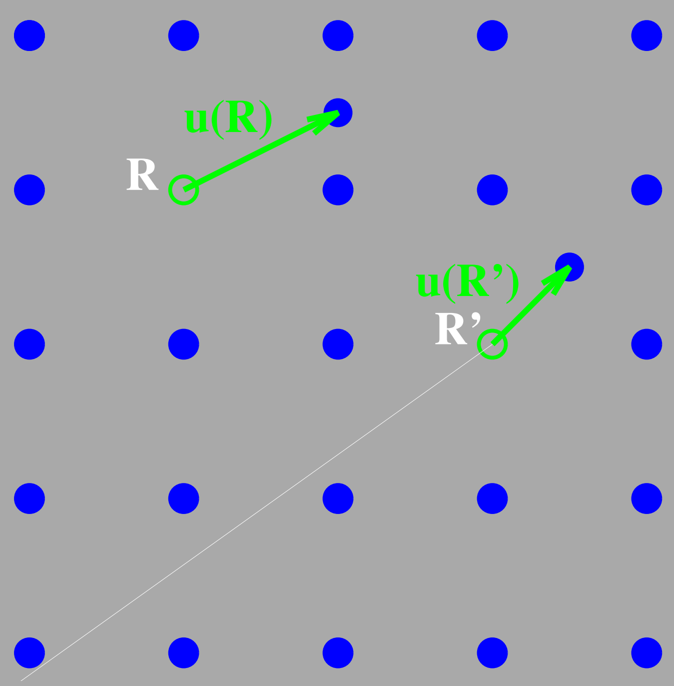
$$+ \cdots$$

lattice dynamics



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$$-\frac{\partial \mathbf{F}(\mathbf{R})}{\partial \mathbf{u}(\mathbf{R}')}$$

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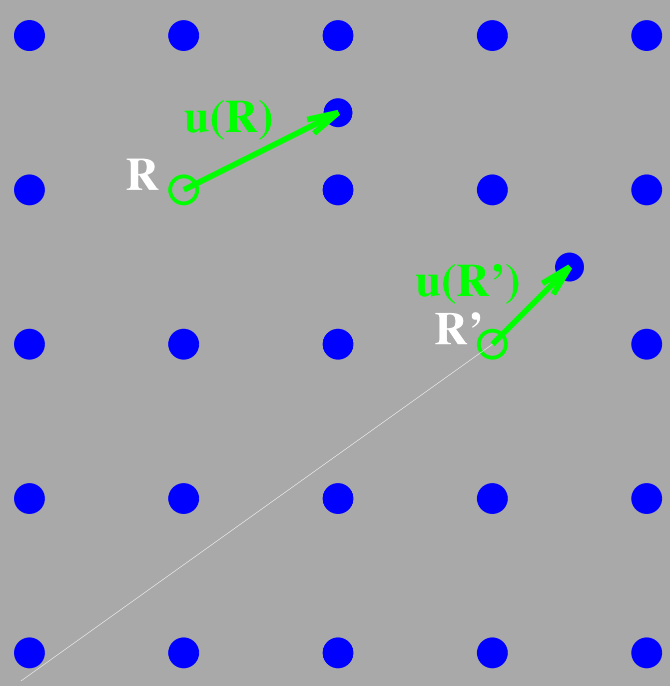
$$+ \cdots$$

lattice dynamics



$$V(\mathbf{r}) = V_0(\mathbf{r}) + \sum_{\mathbf{R}} \mathbf{u}(\mathbf{R}) \cdot \frac{\partial v(\mathbf{r}-\mathbf{R})}{\partial \mathbf{R}} + \cdots$$

DFT

DPFT

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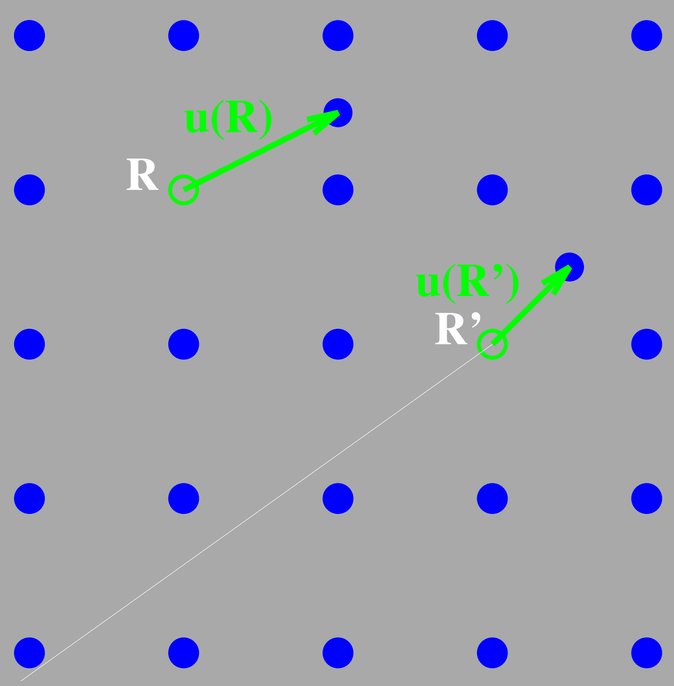
$$+ \cdots$$

lattice dynamics



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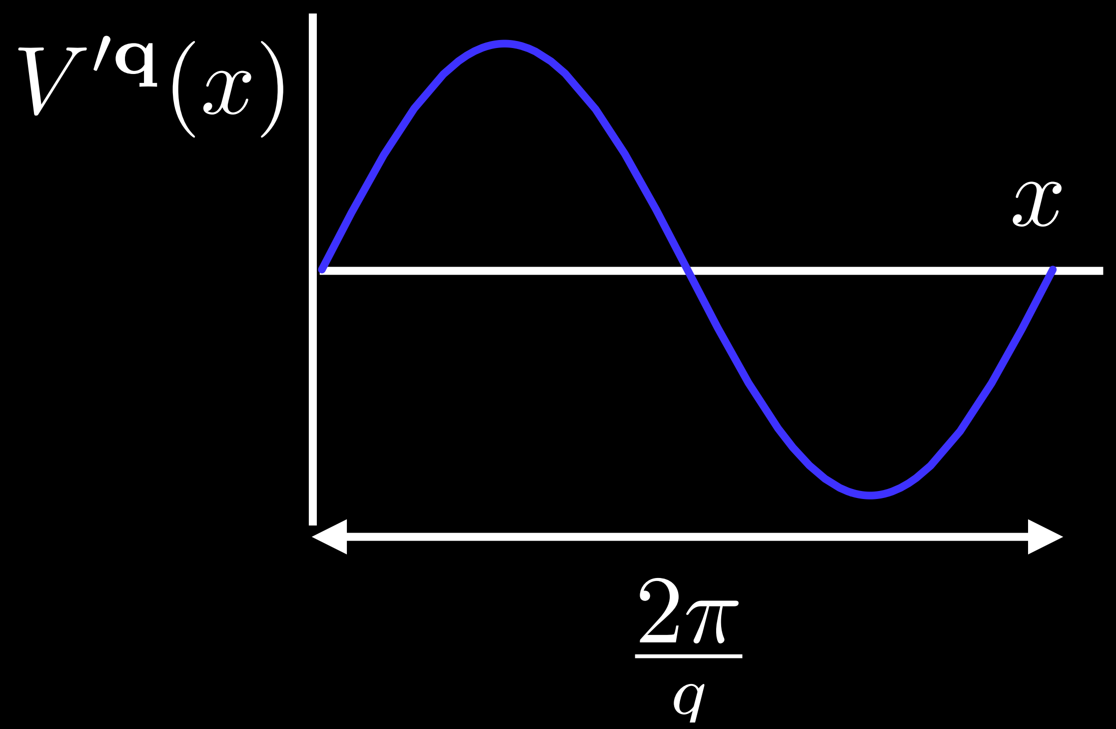
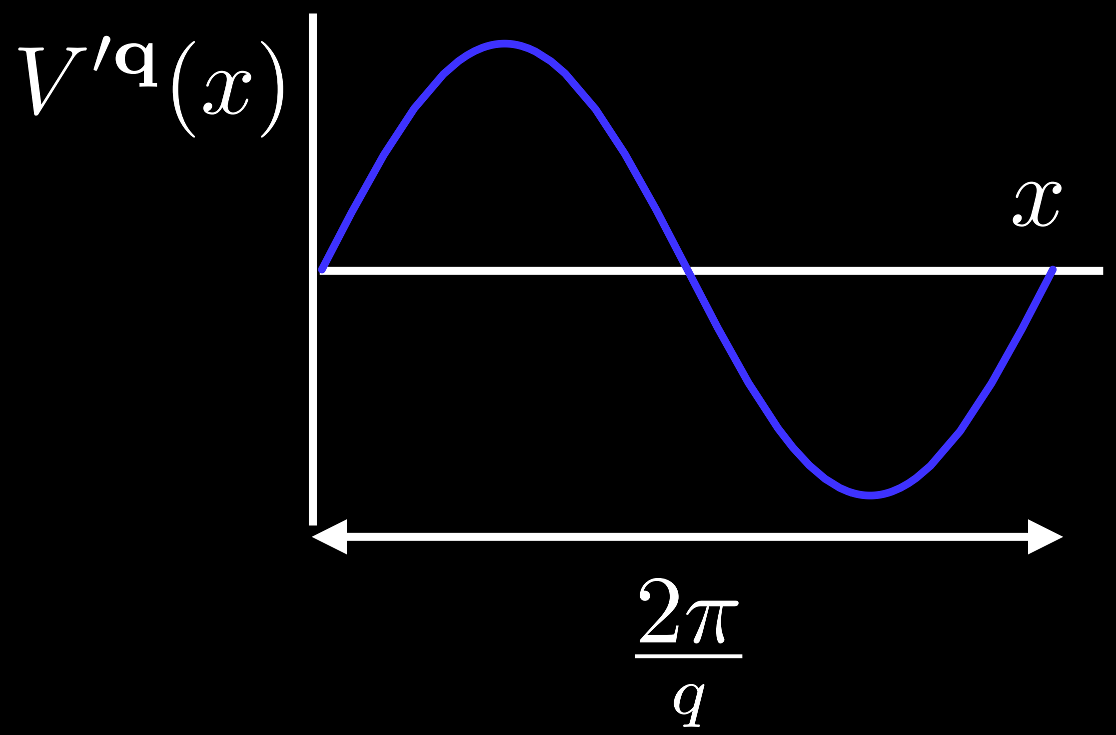
$$\det \left[\frac{\partial^2 E}{\partial \mathbf{u}(\mathbf{R}) \partial \mathbf{u}(\mathbf{R}')} - \omega^2 M(\mathbf{R}) \delta_{\mathbf{R},\mathbf{R}'} \right] = 0$$

monochromatic perturbations



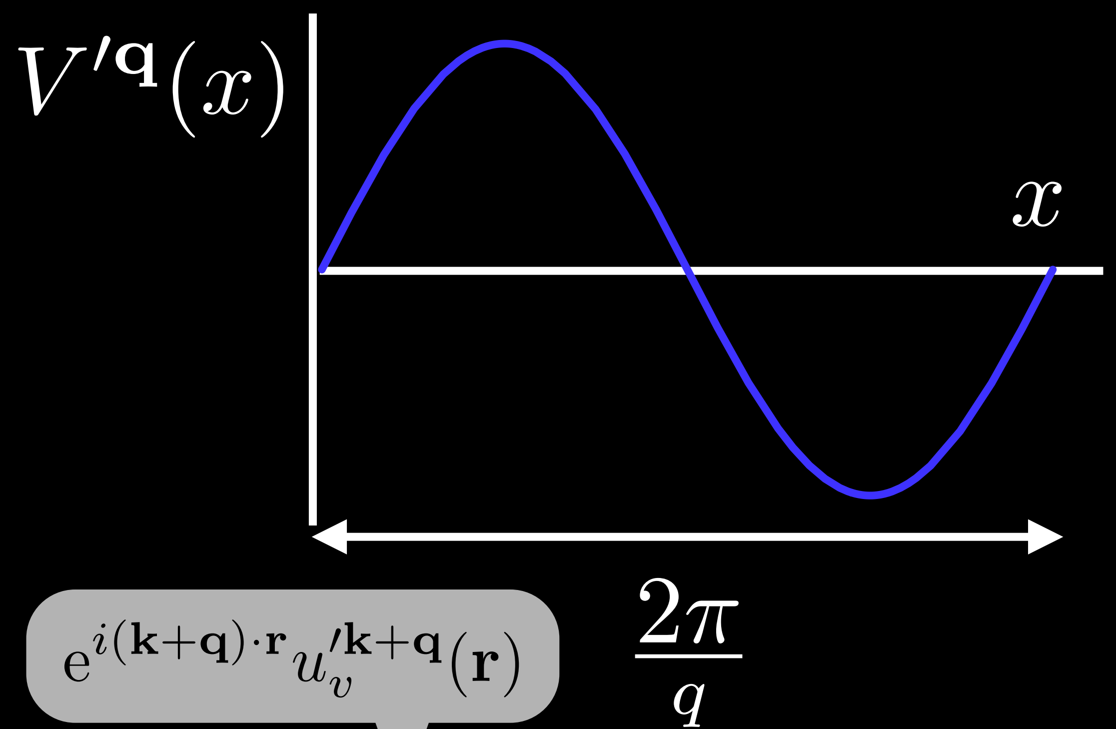
DFPT rhs: $-P_c V'^{\mathbf{q}}_{SCF} \phi^{\mathbf{k}}_v(\mathbf{r})$

monochromatic perturbations



$$\left(H_0 - \epsilon_v^{\mathbf{k}}\right)\phi_v'^{\mathbf{k}+\mathbf{q}}(\mathbf{r}) = -P_c V'^{\mathbf{q}}_{SCF}\phi_v^{\mathbf{k}}(\mathbf{r})$$

monochromatic perturbations

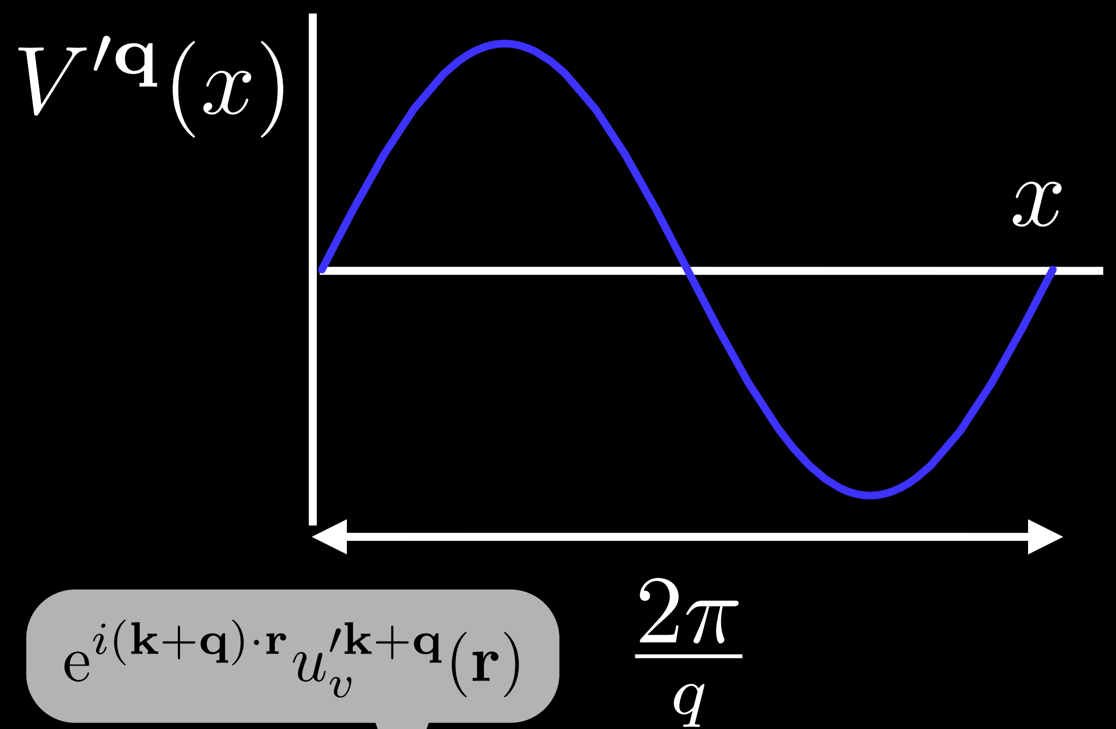


$\mathrm{e}^{i(\mathbf{k}+\mathbf{q})\cdot\mathbf{r}} u_v'^{\mathbf{k}+\mathbf{q}}(\mathbf{r})$

$\mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}} u_v^{\circ\mathbf{k}}(\mathbf{r})$

$$\left(H_0 - \epsilon_v^{\mathbf{k}}\right)\phi_v'^{\mathbf{k}+\mathbf{q}}(\mathbf{r}) = -P_c V_{SCF}'^{\mathbf{q}} \phi_v^{\mathbf{k}}(\mathbf{r})$$

monochromatic perturbations



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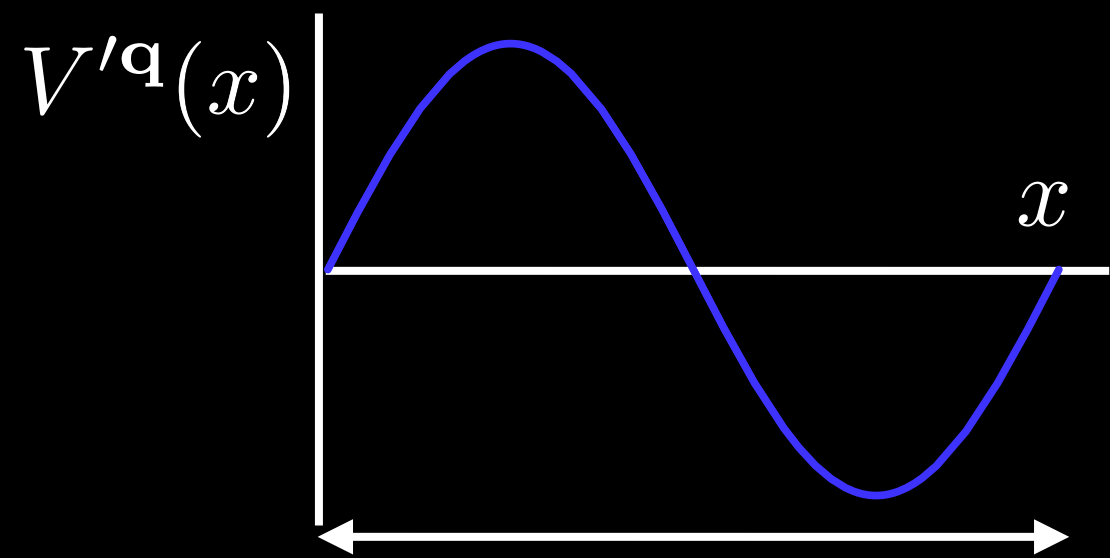
$\mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}}u_v^{\circ\mathbf{k}}(\mathbf{r})$

$$\left(H_0-\epsilon_v^{\mathbf{k}}\right)\phi_v'^{\mathbf{k}+\mathbf{q}}(\mathbf{r})=-P_cV'^{\mathbf{q}}_{SCF}\phi_v^{\mathbf{k}}(\mathbf{r})$$

$$n'^{\mathbf{q}}(\mathbf{r})=\mathrm{e}^{i\mathbf{q}\cdot\mathbf{r}}\sum_{v,\mathbf{k}}u_v^{\circ\mathbf{k}*}(\mathbf{r})u_v'^{\mathbf{k}+\mathbf{q}}(\mathbf{r})$$

monochromatic perturbations



$$\frac{2\pi}{q}$$

$$\mathrm{e}^{i(\mathbf{k}+\mathbf{q})\cdot\mathbf{r}}u_v'^{\mathbf{k}+\mathbf{q}}(\mathbf{r}) \qquad \mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}}u_v^{\circ\mathbf{k}}(\mathbf{r})$$

$$\left(H_0-\epsilon_v^{\mathbf{k}}\right)\phi_v'^{\mathbf{k}+\mathbf{q}}(\mathbf{r})=-P_cV_{SCF}'^{\mathbf{q}}\phi_v^{\mathbf{k}}(\mathbf{r})$$

$$n'^{\mathbf{q}}(\mathbf{r})=\mathrm{e}^{i\mathbf{q}\cdot\mathbf{r}}\sum_{v,\mathbf{k}}u_v^{\circ\mathbf{k}*}(\mathbf{r})u_v'^{\mathbf{k}+\mathbf{q}}(\mathbf{r})$$

$$V'^{\mathbf{q}}(\mathbf{r})=V_{ext}'^{\mathbf{q}}(\mathbf{r})+\int\left(\frac{e^2}{|\mathbf{r}-\mathbf{r}'|}+\kappa_{xc}(\mathbf{r},\mathbf{r}')\right)n'^{\mathbf{q}}(\mathbf{r}')d\mathbf{r}'$$

phonons in polar materials

$$E(\mathbf{u} \quad) = \frac{1}{2} M\omega_0^2 u^2$$

phonons in polar materials

$$E(\mathbf{u}, \mathsf{E}) = \frac{1}{2} M \omega_0^2 u^2 - \frac{\Omega}{8\pi} \epsilon_\infty \mathsf{E}^2 - eZ^* \mathbf{u} \cdot \mathsf{E}$$

phonons in polar materials

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$$\begin{aligned}
\mathbf{F} &\equiv -\frac{\partial E}{\partial \mathbf{u}} = -M\omega_0^2 \mathbf{u} + Z^* \mathsf{E} \\
\mathsf{D} &\equiv -\frac{4\pi}{\Omega} \frac{\partial E}{\partial \mathsf{E}} = \frac{4\pi}{\Omega} Z^* \mathbf{u} + \epsilon_\infty \mathsf{E}
\end{aligned}$$

phonons in polar materials

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$$\mathrm{rot}\ \mathsf{E} \sim i\mathbf{q}\times\mathsf{E} = 0$$

phonons in polar materials

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\mathsf{D} &\equiv -\frac{4\pi}{\Omega}\frac{\partial E}{\partial \mathsf{E}} = \frac{4\pi}{\Omega}Z^*\mathbf{u} + \epsilon_\infty\mathsf{E}
\end{aligned}$$

$\mathrm{rot}\ \mathsf{E} \sim i\mathbf{q}\times\mathsf{E} = 0$ $\qquad$ $\mathbf{u}\perp\mathbf{q} \Rightarrow \mathsf{E} = 0$ $\qquad$ (T)

phonons in polar materials

$$E(\mathbf{u},\mathsf{E}) = \frac{1}{2}M\omega_0^2u^2 - \frac{\Omega}{8\pi}\epsilon_\infty\mathsf{E}^2 - eZ^*\mathbf{u}\cdot\mathsf{E}$$

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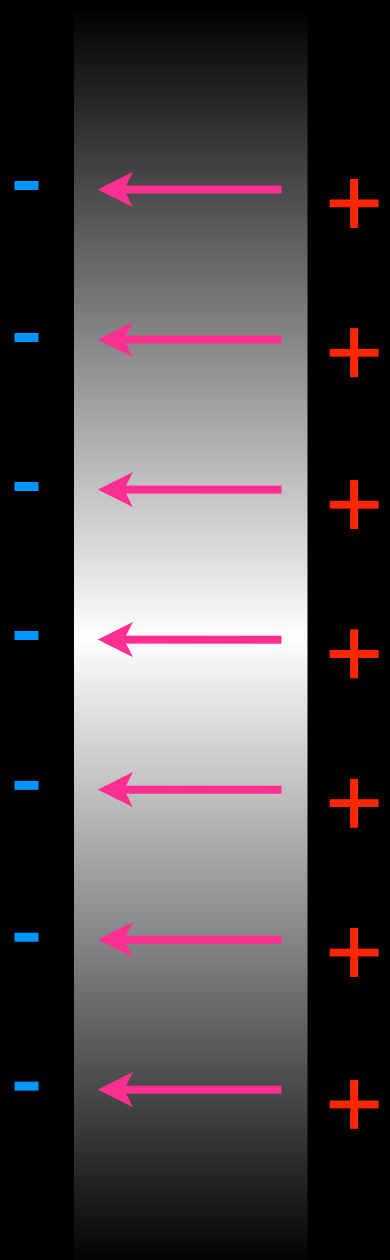
$\mathbf{F}_T = -M\omega_0^2 \mathbf{u}$ $\qquad$ $\mathbf{F}_L = -M\left(\omega_0^2 + \frac{4\pi Z^*}{M\Omega\epsilon_\infty}\right)\mathbf{u}$

macroscopic electric fields

$\mathbf{E} = \text{const}$



$V'(\mathbf{r}) = \mathbf{E} \cdot \mathbf{r}$

macroscopic electric fields

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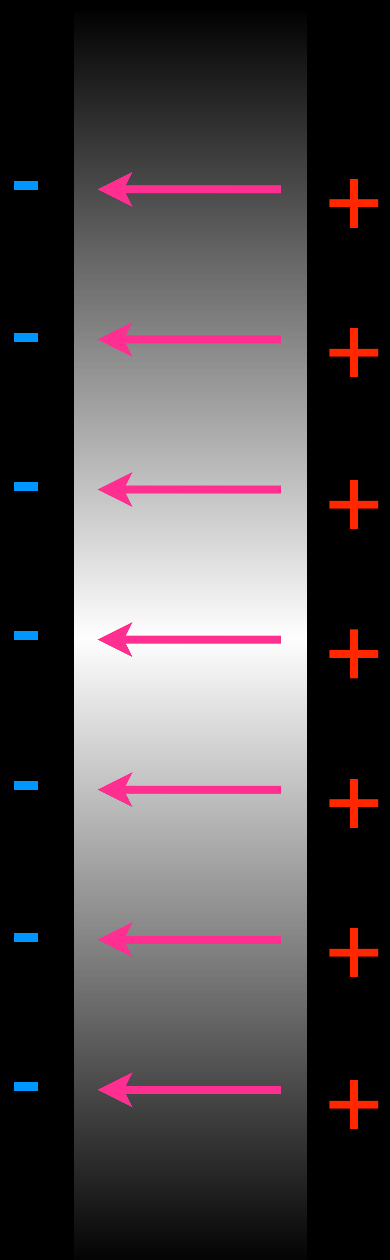

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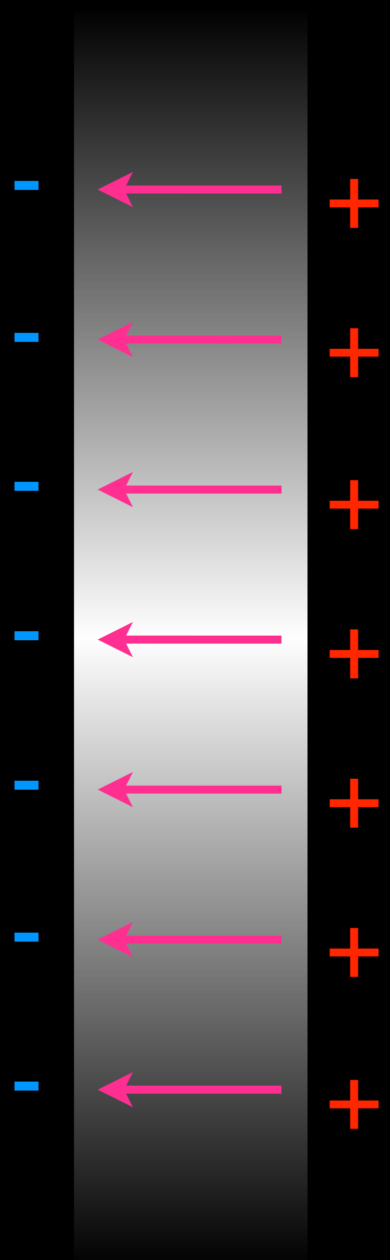

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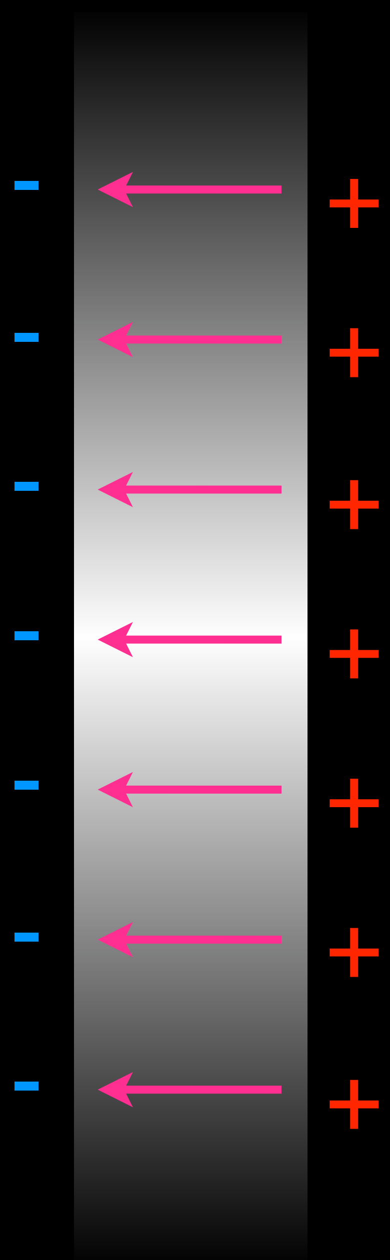

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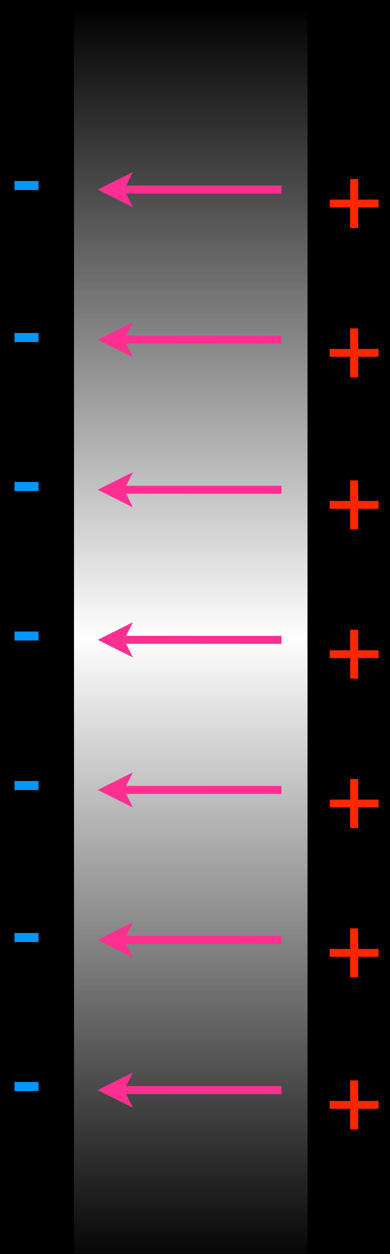

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$$\langle \phi_v^0 | x | \phi_u^0 \rangle = \frac{\langle \phi_v^0 | [H, x] | \phi_u^0 \rangle}{\epsilon_v^0 - \epsilon_u^0} \qquad [H, x] = -\frac{\hbar^2}{m}\frac{\partial}{\partial x} + [H, V_{nl}]$$

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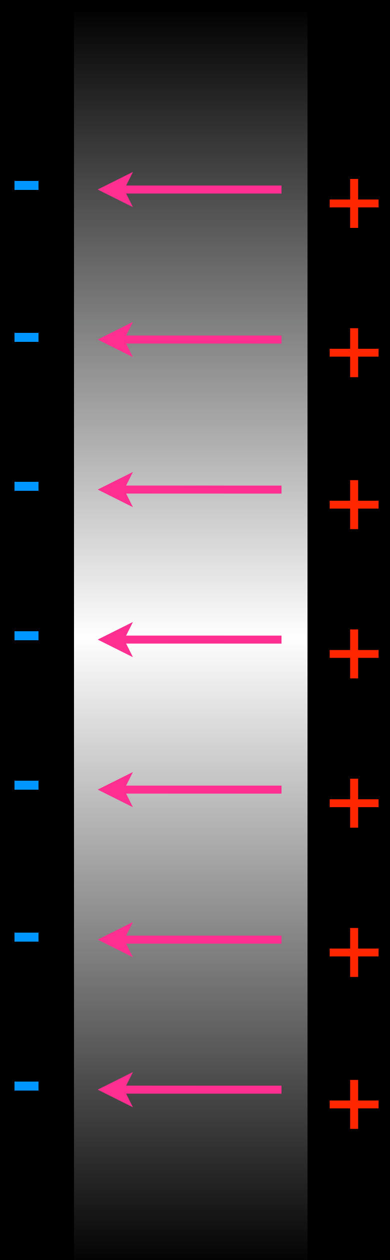

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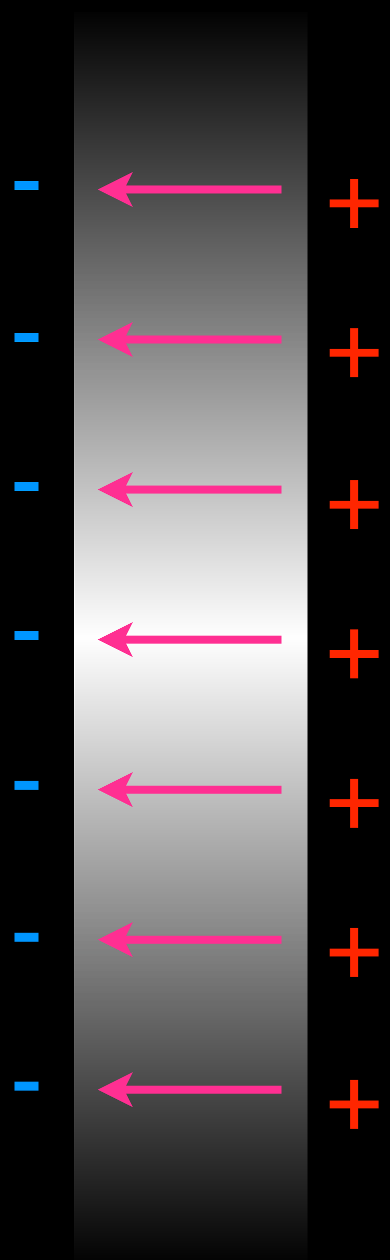
macroscopic electric fields

$\mathsf{E} = \mathrm{const}$



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$V'(\mathbf{r}) = \mathsf{E} \cdot \mathbf{r}$

$$\boxed{(H_0 - \epsilon_v^0)\psi_v' = -\mathsf{E} P_c [H_0, x] \phi_v^0}$$

DFPT rhs

interatomic force constants

$$\Phi_{st}^{\alpha\beta}(\mathbf{R}-\mathbf{R}') \quad = \quad -\frac{\partial^2 E}{\partial u_s^\alpha(\mathbf{R})\partial u_t^\beta(\mathbf{R}')}$$

interatomic force constants

$$\begin{aligned}
\Phi_{st}^{\alpha\beta}(\mathbf{R}-\mathbf{R}') &= -\frac{\partial^2 E}{\partial u_s^\alpha(\mathbf{R})\partial u_t^\beta(\mathbf{R}')} \\
&= \frac{\Omega}{(2\pi)^3}\int \mathrm{e}^{i\mathbf{q}\cdot(\mathbf{R}-\mathbf{R}')} D_{st}^{\alpha\beta}(\mathbf{q}) d\mathbf{q}
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short ranged +
dipole-dipole

interatomic force constants

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short ranged +
dipole-dipole

- **remove singularities** in D(q)
- **do FFT's** (# R's = # q's - the shorter the range, the coarser the grid)
- **store information**
- **interpolate** D(q) on any finer mesh (pad Φ with 0's and do FFT^{-1}: # q's = # R's)
- **calculate phonon bands**

DFPT: the main features

- ☛ response functions calculated in terms of response orbitals, $\{\phi'_v\}$

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- non-local perturbations: OK
- non-periodic perturbations: OK
- macroscopic electric fields: OK

Piezoelectric Properties of III-V Semiconductors from First-Principles Linear-Response Theory

Stefano de Gironcoli[(a)]
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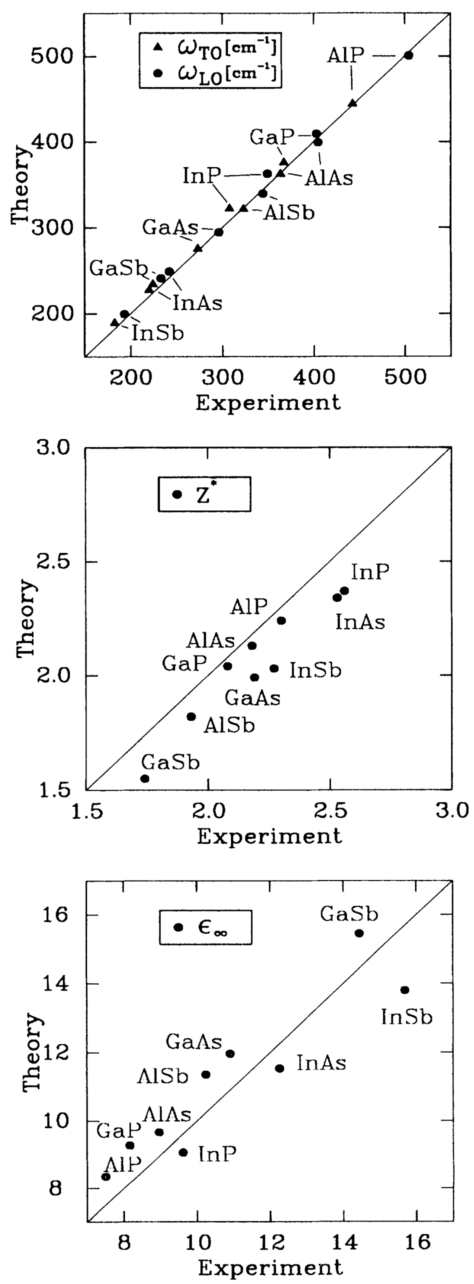
Stefano Baroni
Scuola Internazionale Superiore di Studi Avanzati (SISSA), Strada Costiera 11, I-34014 Trieste, Italy

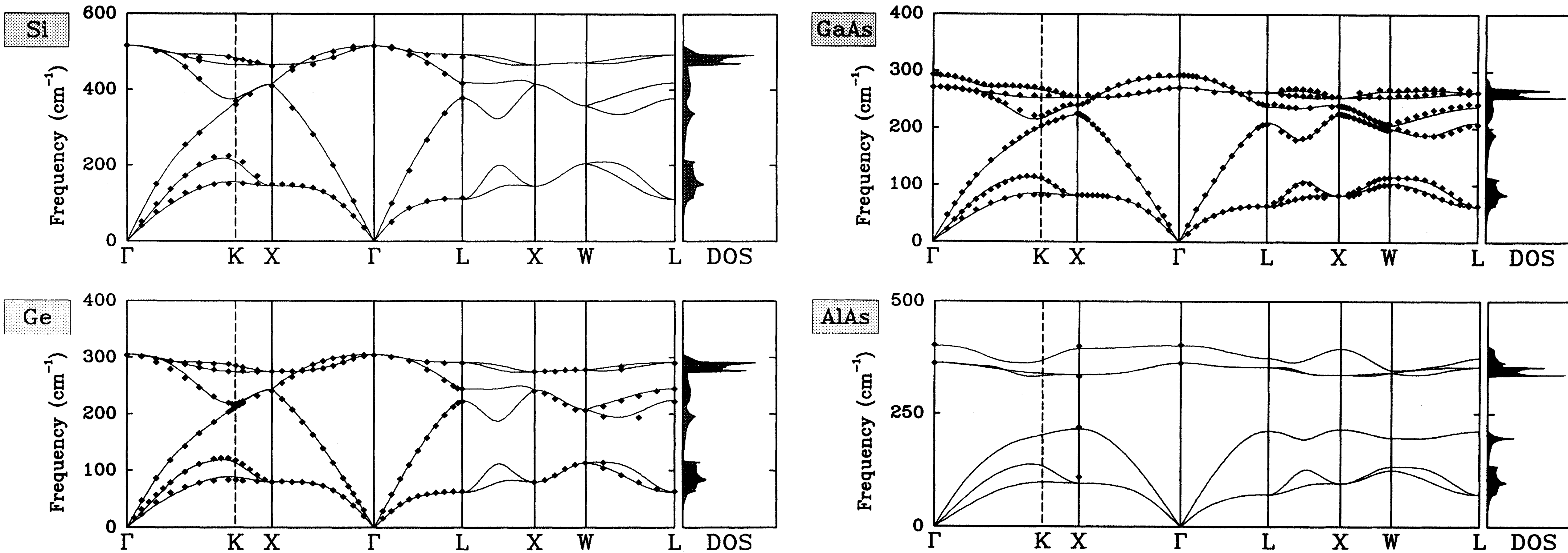
Raffaele Resta[(b)]
Institut Romand de Recherche Numérique en Physique des Matériaux (IRRMA), Ecole Polytechnique Fédérale de Lausanne, CH-1015, Lausanne, Switzerland

(Received 7 November 1988)



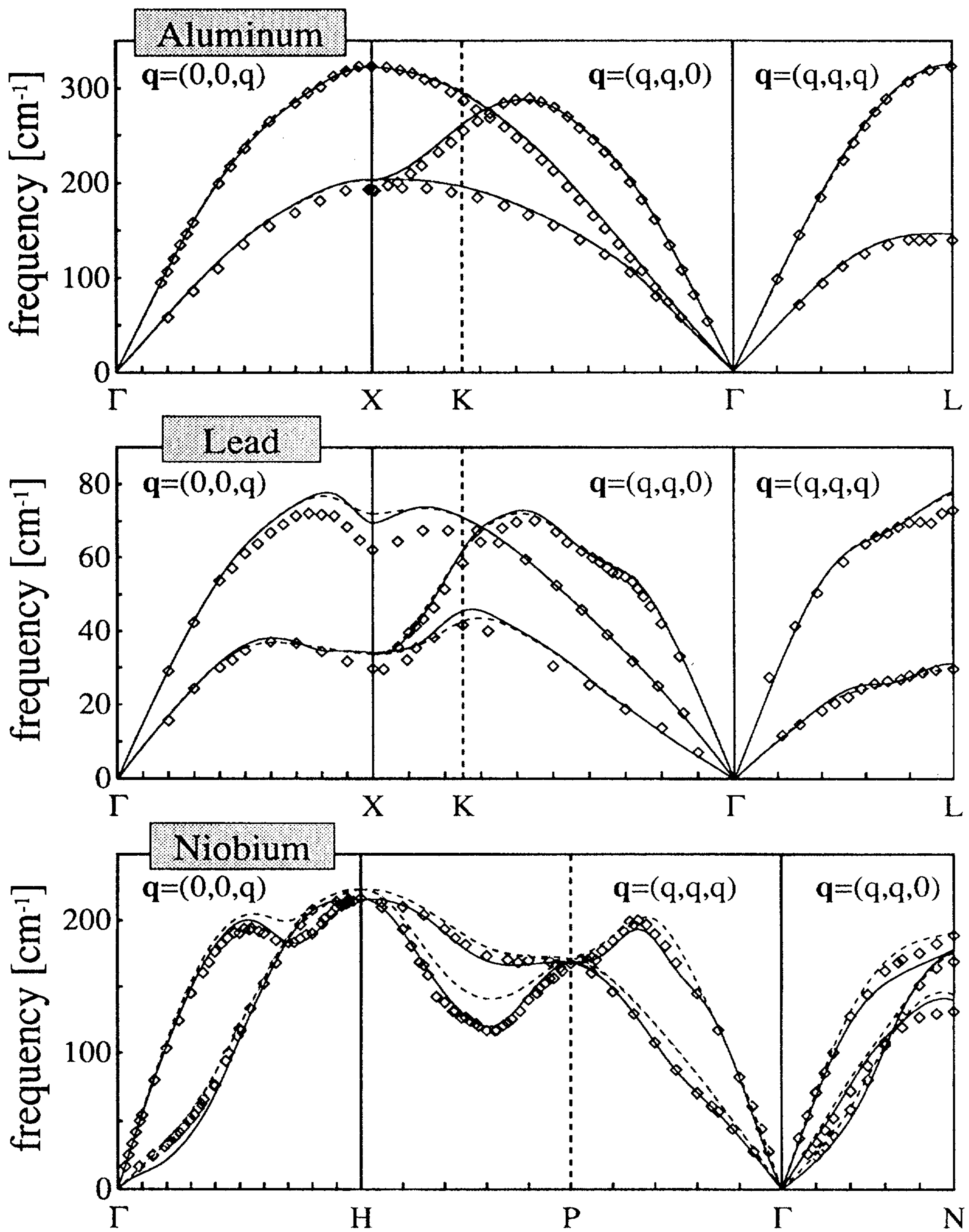
$\bar{\gamma}_{14}$	P	As	Sb
Al	0.11 (· · ·)	−0.03 (· · ·)	−0.13 (−0.16)
Ga	−0.18 (−0.18)	−0.35 (−0.32)	−0.40 (−0.39)
In	0.12 (|0.09|)	−0.08 (−0.10)	−0.20 (−0.18)

phonons from DFPT



P. Giannozzi, S. de Gironcoli, P. Pavone, and SB, Phys. Rev. B **43**, 7231 (1991)

DFPT phonons in metals



Stefano de Gironcoli,
Phys. Rev. B **51**, 6773 (1995)

applications done so far

- Dielectric properties
- Piezoelectric properties
- Elastic properties
- Phonon in crystals and alloys
- Phonon at surfaces, interfaces, super-lattices, and nano-structures
- Raman and infrared activities
- Anharmonic couplings and vibrational line widths
- Mode softening and structural transitions
- Electron-phonon interaction and superconductivity
- Thermal expansion
- Isotopic effects on structural and dynamical properties
- Thermo-elasticity and other thermal properties of minerals
- …

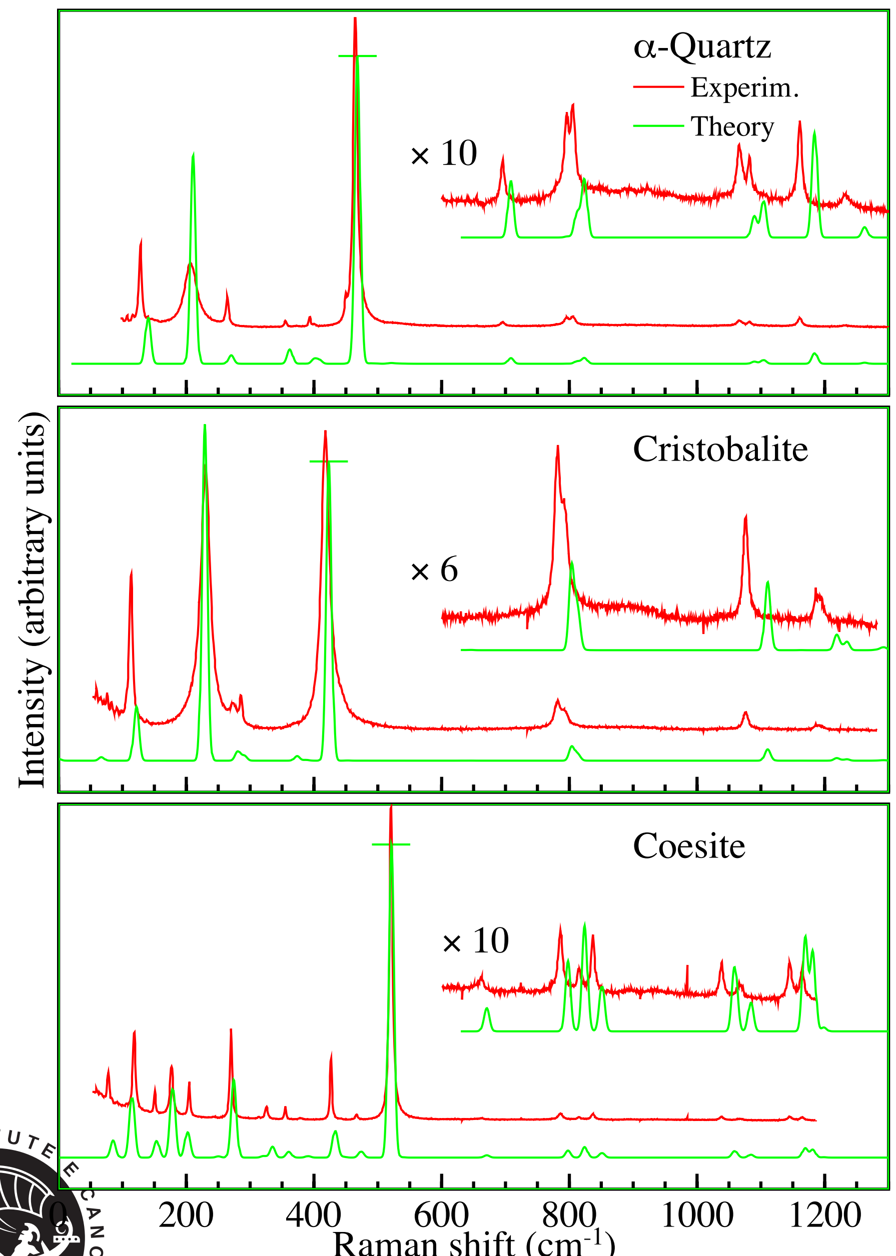
SB, A. Dal Corso, S. de Gironcoli, and P. Giannozzi, *Phonons and related crystal properties from density-functional perturbation theory*, Rev. Mod. Phys. **73**, 515 (2001)

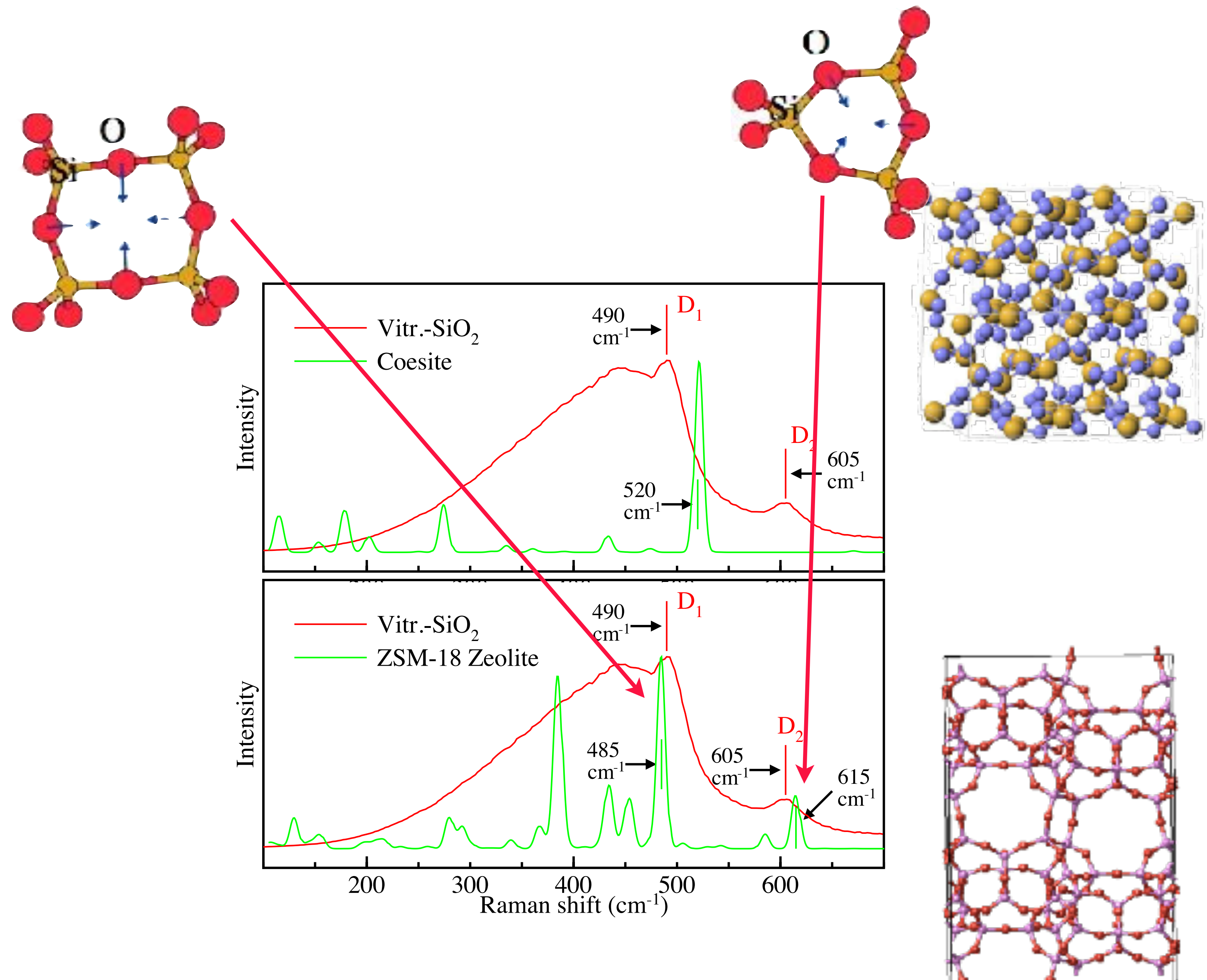
a sampler of recent applications

VOLUME 90, NUMBER 3 PHYSICAL REVIEW LETTERS week ending 24 JANUARY 2003

First-Principles Calculation of Vibrational Raman Spectra in Large Systems: Signature of Small Rings in Crystalline SiO_2

Michele Lazzeri and Francesco Mauri





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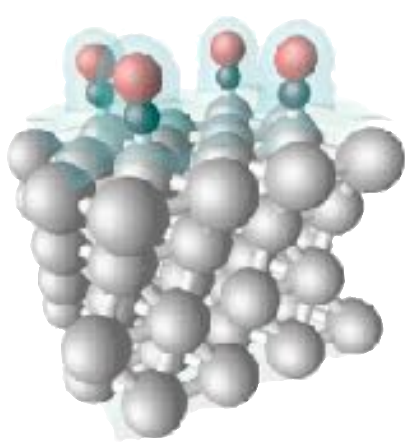
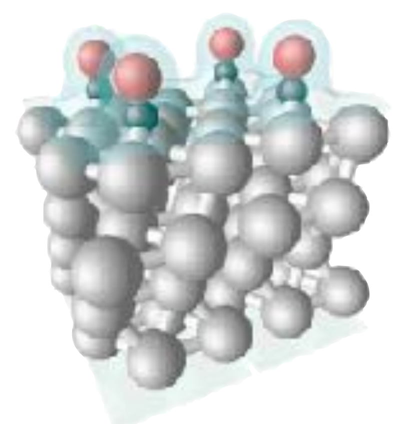
Vibrational Recognition of Adsorption Sites for CO on Platinum and Platinum−Ruthenium Surfaces

Ismaila Dabo,*,† Andrzej Wieckowski,‡ and Nicola Marzari†

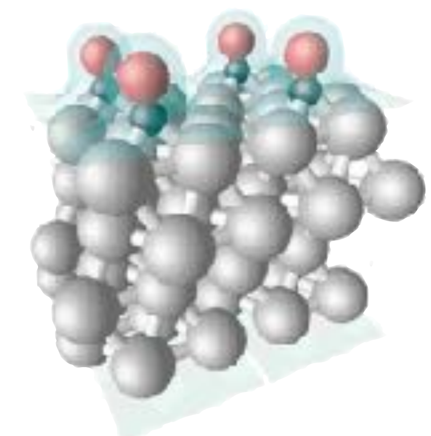
11046 J. AM. CHEM. SOC. ■ VOL. 129, NO. 36, 2007



atop ($CO@Pt_1$)
E_{DFT} = +0.10 eV
ν_{DFT} = 2050 cm^{-1}
ν_{exp} = 2070 cm^{-1}



bridge ($CO@Pt_2$)
E_{DFT} = +0.03 eV
ν_{DFT} = 1845 cm^{-1}
ν_{exp} = 1830 cm^{-1}



fcc ($CO@Pt_3$)
E_{DFT} = 0 eV
ν_{DFT} = 1743 cm^{-1}
ν_{exp} = 1780 cm^{-1}

expt

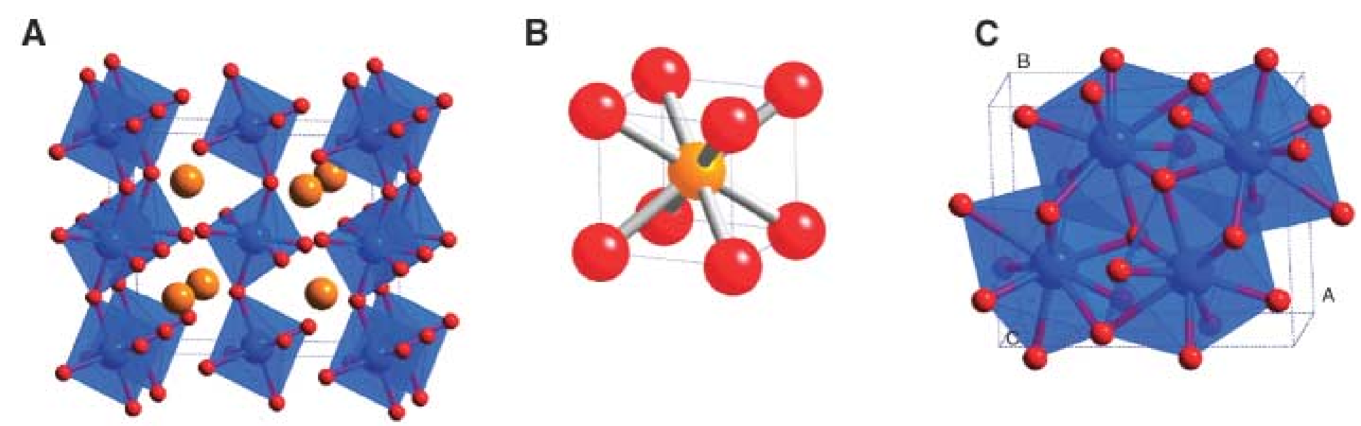
DFT

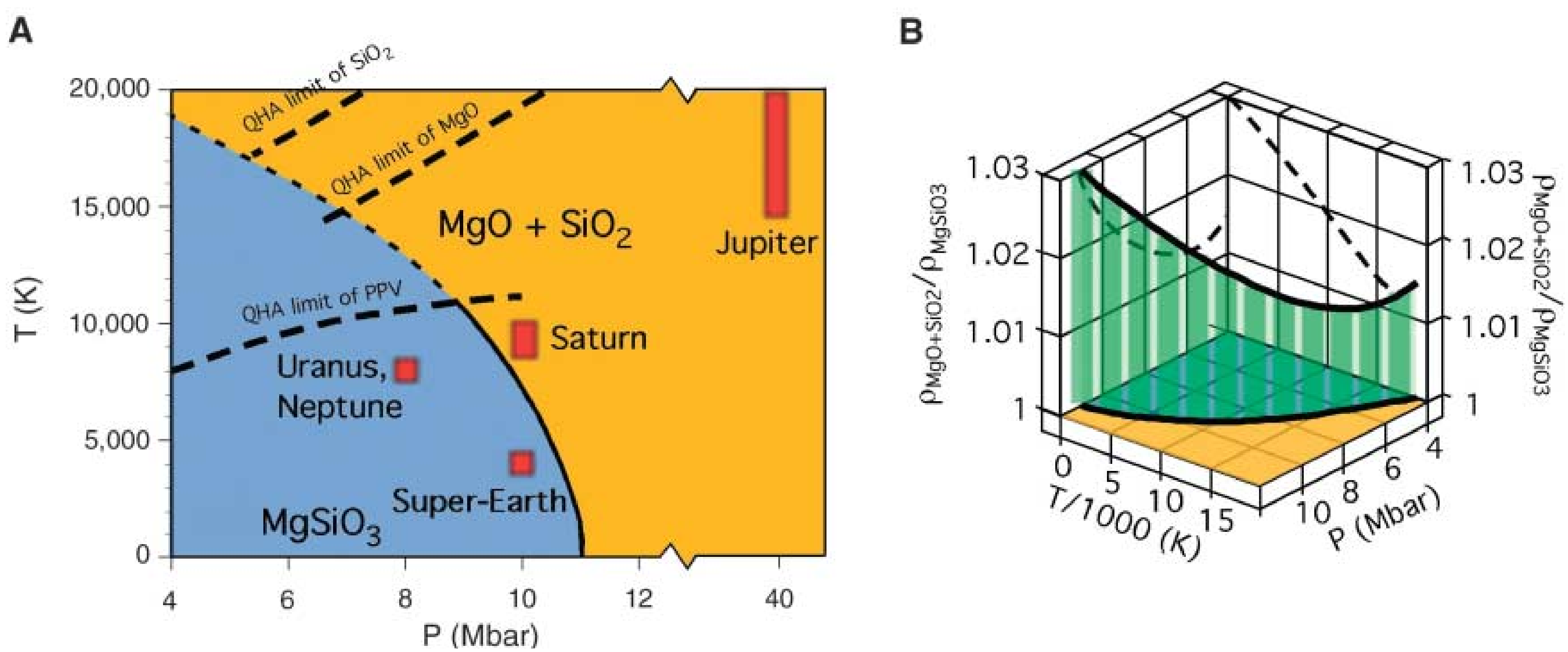
a sampler of recent applications

Dissociation of $MgSiO_3$ in the Cores of Gas Giants and Terrestrial Exoplanets

Koichiro Umemoto,[1] Renata M. Wentzcovitch,[1*] Philip B. Allen[2]

www.sciencemag.org SCIENCE VOL 311 17 FEBRUARY 2006 983





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PRL **100,** 257001 (2008) PHYSICAL REVIEW LETTERS week ending 27 JUNE 2008

Ab Initio Description of High-Temperature Superconductivity in Dense Molecular Hydrogen

P. Cudazzo,[1] G. Profeta,[1] A. Sanna,[2,3] A. Floris,[3] A. Continenza,[1] S. Massidda,[2] and E. K. U. Gross[3]

[1]*CNISM - Dipartimento di Fisica, Università degli Studi dell'Aquila, Via Vetoio 10, I-67010 Coppito (L'Aquila) Italy*
[2]*SLACS-INFM/CNR—Dipartimento di Fisica, Università degli Studi di Cagliari, I-09124 Monserrato (CA), Italy*
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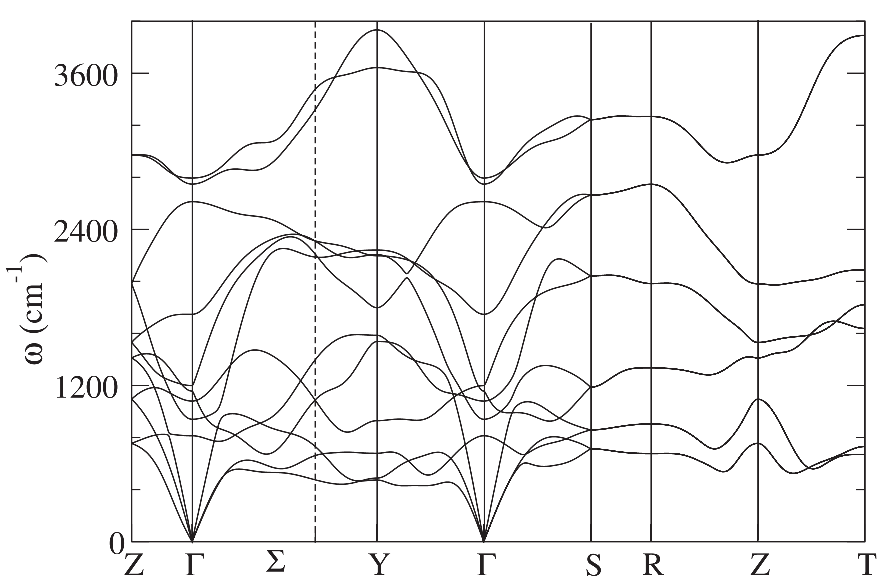
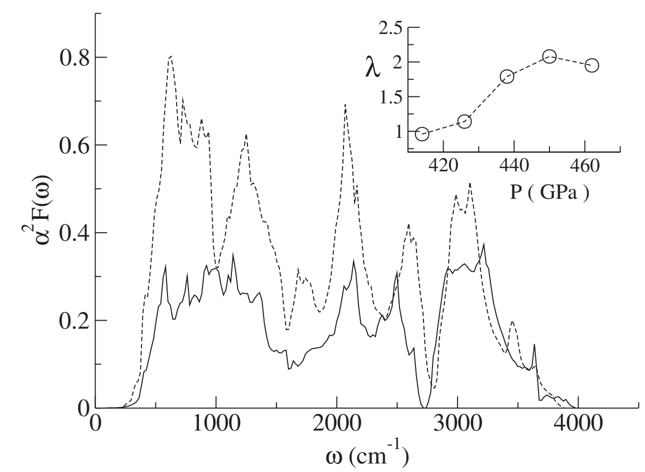
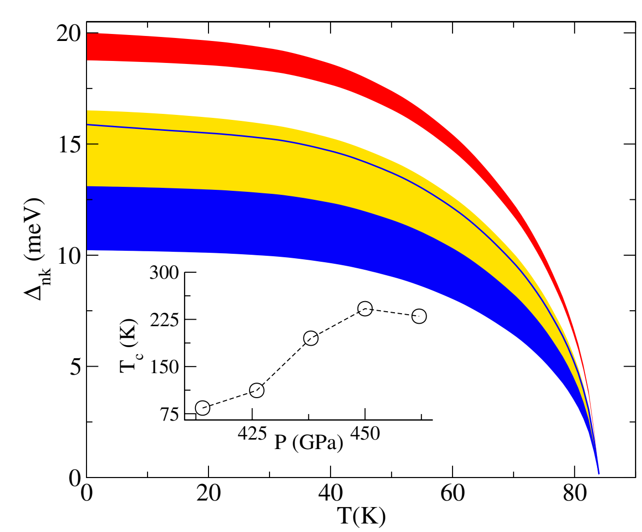
(Received 7 December 2007; published 23 June 2008; corrected 27 June 2008)

414 GPa







a sampler of recent applications

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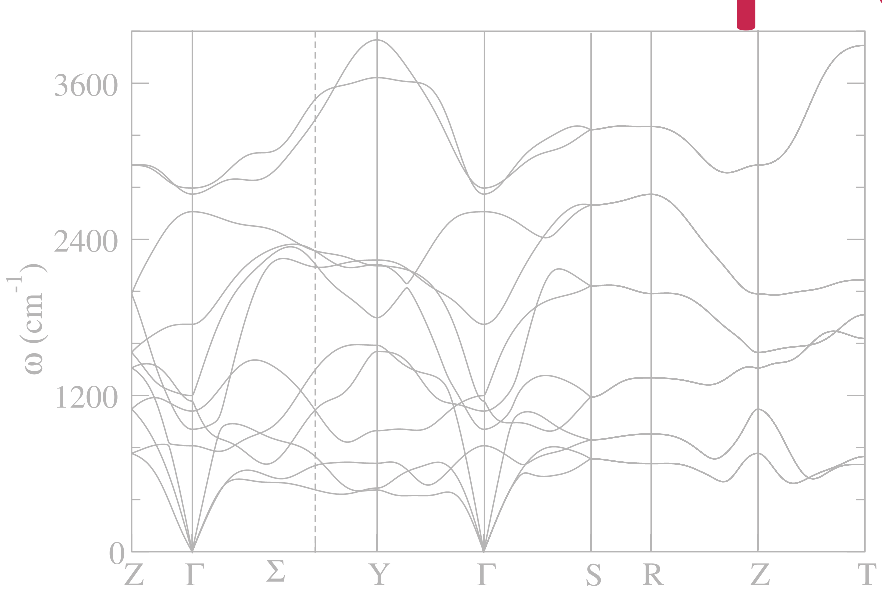
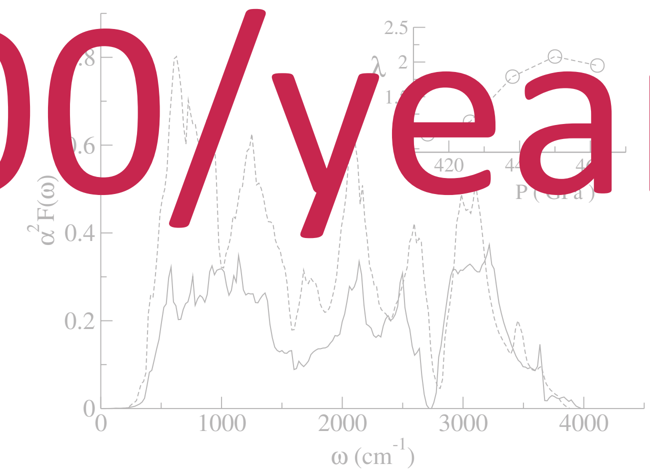
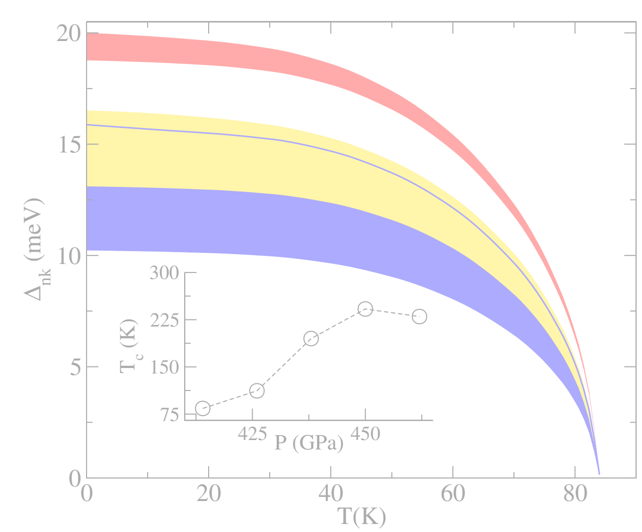
414 GPa

$\cdots + \approx 400/\text{year}$







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MAX

MA PER SEGUIR VIRTUTE E CANOSCENZA

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http://talks.baroni.me