density-functional perturbation theory

response functions, phonons, and all that

Stefano Baroni

Scuola Internazionale Superiore di Studi Avanzati
Trieste - Italy

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response functions

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

response functions

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

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

the Hellmann-Feynman theorem

$$\hat{H}_\lambda \Psi_\lambda = E_\lambda \Psi_\lambda$$

the Hellmann-Feynman theorem

$$\hat{H}_\lambda \Psi_\lambda = E_\lambda \Psi_\lambda \qquad E'_\lambda = \frac{\partial}{\partial \lambda} \langle \Psi_\lambda | \hat{H}_\lambda | \Psi_\lambda \rangle$$

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$$= \langle \Psi_\lambda | \hat{H}_\lambda | \Psi_\lambda \rangle + \langle \Psi_\lambda | \hat{H}'_\lambda | \Psi_\lambda \rangle + \langle \Psi_\lambda | \hat{H}_\lambda | \Psi'_\lambda \rangle$$

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$$E_\lambda = \min_{\{\Psi:\ \langle \Psi | \Psi \rangle = 1\}} \langle \Psi | \hat{H}_\lambda | \Psi \rangle$$

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$$g(\lambda) = \min_x G[x, \lambda]$$

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$$g(\lambda) = G[x(\lambda), \lambda] \longrightarrow g'(\lambda) = x'(\lambda) \left. \frac{\partial G}{\partial x} \right|_{x = x(\lambda)} + \frac{\partial G}{\partial \lambda}$$

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the Hellmann-Feynman theorem

$$\hat{H}_\lambda \Psi_\lambda = E_\lambda \Psi_\lambda$$

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$$\hat{H}_\lambda \Psi_\lambda = E_\lambda \Psi_\lambda$$

$$E'_\lambda = \langle \Psi_\lambda | \hat{H}'_\lambda | \Psi_\lambda \rangle$$

$$\frac{\partial}{\partial \lambda} \min_x G(x,\lambda) = \left. \frac{\partial G(x,\lambda)}{\partial \lambda} \right|_{x=x(\lambda)}$$

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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

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

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

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

(Hellmann & Feynman)

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

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

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

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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
  - ...

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

$$V_\lambda(\mathbf{r}) = V_0(\mathbf{r}) + \sum_i \lambda_i v_i(\mathbf{r})$$

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

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

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

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

the “2n+1” theorem

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

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$$\Phi = \Phi_0 + \sum_{l=1}^{n} \lambda^l \Phi^{(l)} + \mathcal{O}(\lambda^{n+1})$$

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$$E = E_0 + \sum_{l=1}^{2n+1} \lambda^l E^{(l)} + \mathcal{O}(\lambda^{2n+2})$$

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

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the "2n+1" theorem

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

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

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

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

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

$$= 2\mathrm{Re} \sum_{cv} \rho'_{vc} \phi_v^{\circ *}(\mathbf{r}) \phi_c^{\circ}(\mathbf{r})$$

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

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

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calculating the response

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

$$(H^\circ - \epsilon_v^\circ)\phi_v' = -P_c V' \phi_v^\circ$$

DFPT: the equations

DFT

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

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

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

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

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DFPT: the equations

DFT	DFPT
$V_0(\mathbf{r}) \leftrightarrows n(\mathbf{r})$	$V'(\mathbf{r}) \leftrightarrows n'(\mathbf{r})$

DFT

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

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

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

DFPT

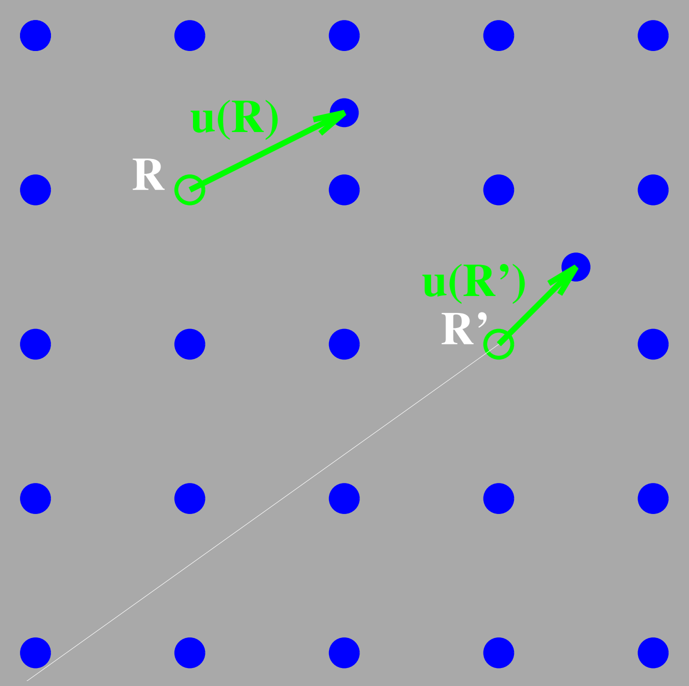
$$V'_{SCF}(\mathbf{r}) = V'(\mathbf{r}) + \int \frac{n'(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} d\mathbf{r}' + \mu'_{xc}(\mathbf{r})$$

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

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

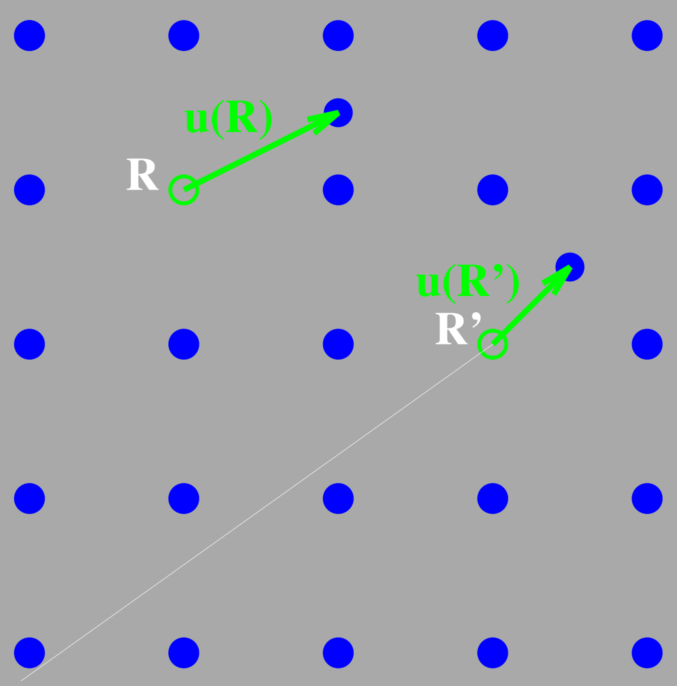
SB, P. Giannozzi, and A. Testa, Phys. Rev. Lett. **58**, 1861 (1987) simulating atomic vibrations …

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

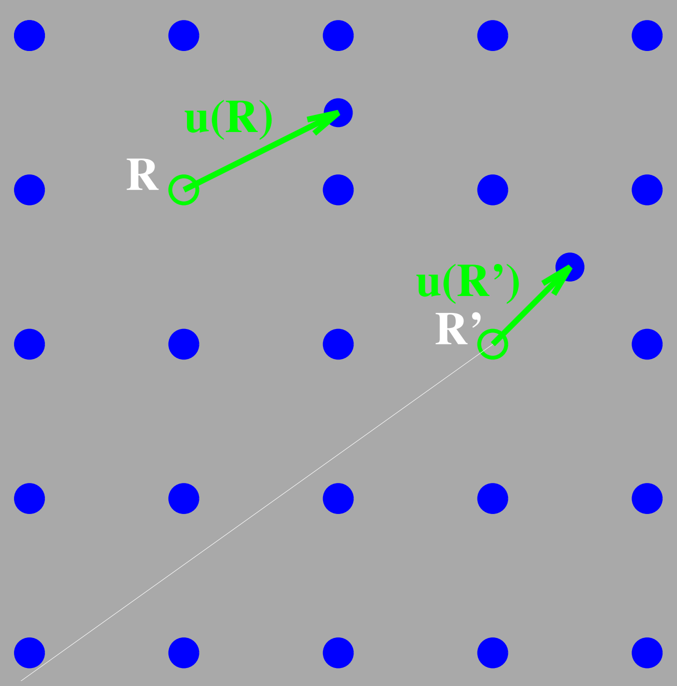


$$V(\mathbf{r}) = V_0(\mathbf{r}) + \sum_{\mathbf{R}} \mathbf{u}(\mathbf{R}) \cdot \frac{\partial v(\mathbf{r}-\mathbf{R})}{\partial \mathbf{R}} + \cdots$$

$$E = E_0 + \frac{1}{2} \sum_{\mathbf{R},\mathbf{R}'} \mathbf{u}(\mathbf{R}) \cdot \frac{\partial^2 E}{\partial \mathbf{u}(\mathbf{R}) \partial \mathbf{u}(\mathbf{R}')} \cdot \mathbf{u}(\mathbf{R}')$$

$$+ \cdots$$

lattice dynamics



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

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

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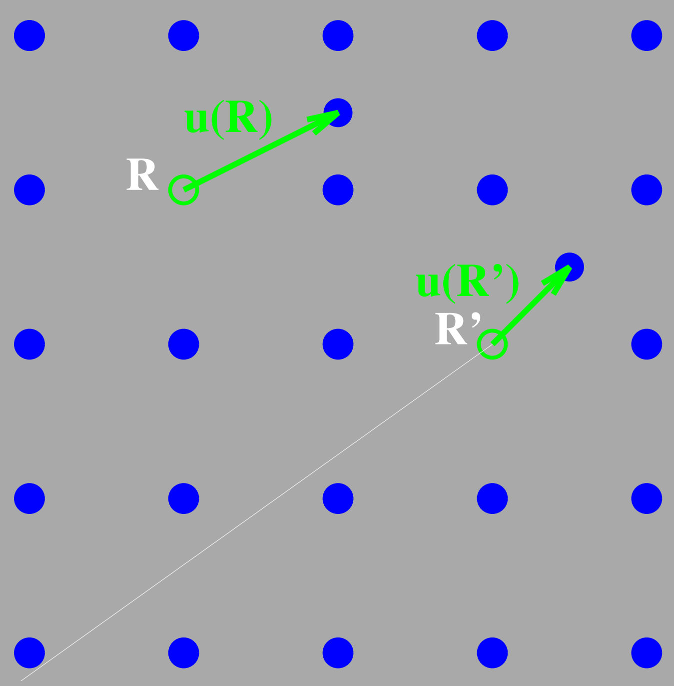
$$+ \cdots$$

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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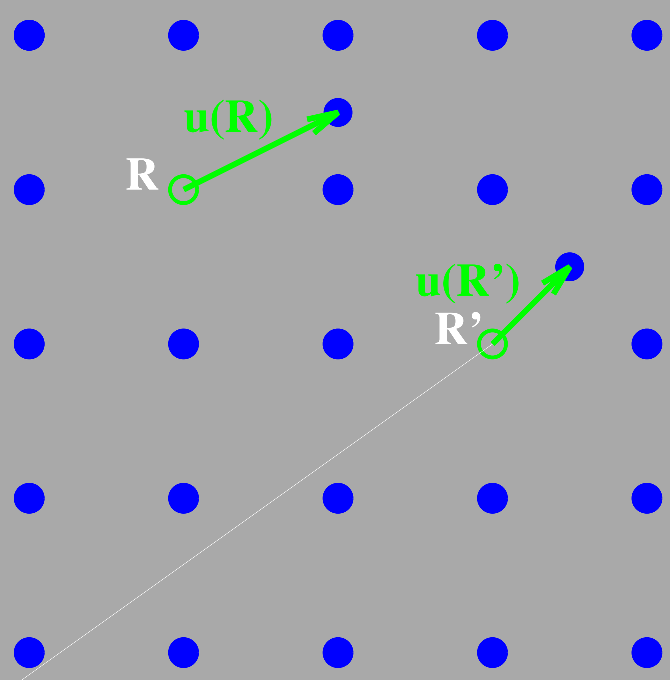
$$E = E_0 + \frac{1}{2}\sum_{\mathbf{R},\mathbf{R}'} \mathbf{u}(\mathbf{R}) \cdot \frac{\partial^2 E}{\partial \mathbf{u}(\mathbf{R})\partial \mathbf{u}(\mathbf{R}')} \cdot \mathbf{u}(\mathbf{R}')$$

$$+\cdots$$

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

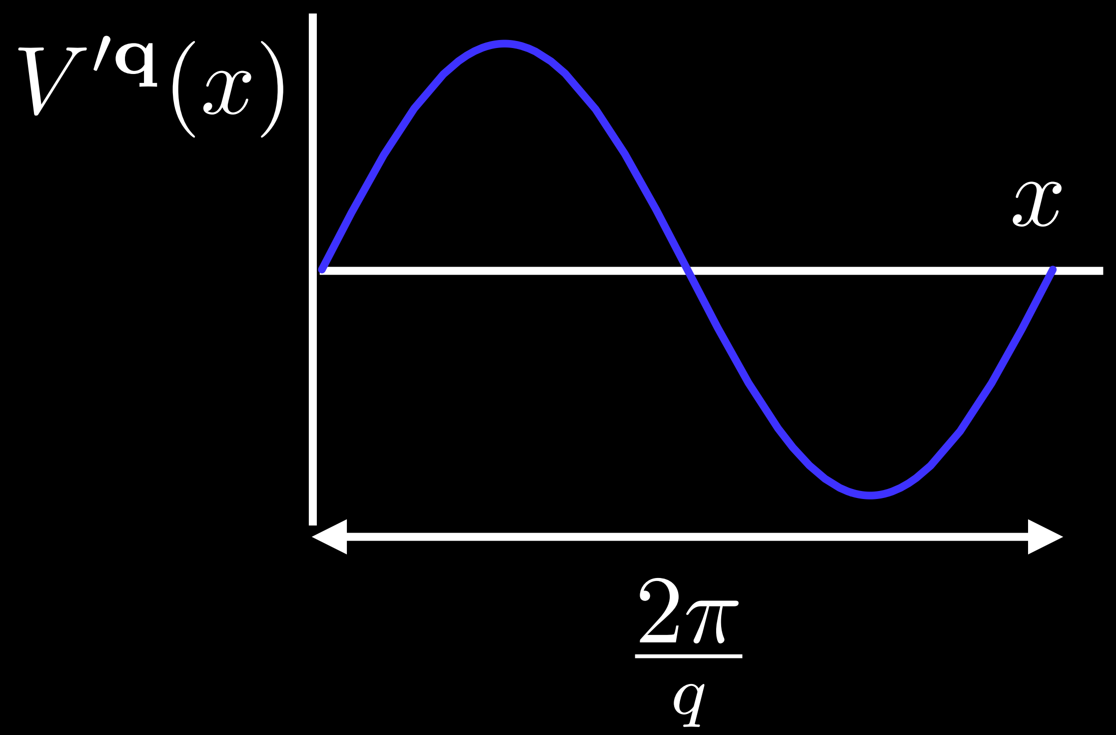
$$-\frac{\partial \mathbf{F}(\mathbf{R})}{\partial \mathbf{u}(\mathbf{R}')}$$

$$E = E_0 + \frac{1}{2} \sum_{\mathbf{R},\mathbf{R}'} \mathbf{u}(\mathbf{R}) \cdot \frac{\partial^2 E}{\partial \mathbf{u}(\mathbf{R}) \partial \mathbf{u}(\mathbf{R}')} \cdot \mathbf{u}(\mathbf{R}')$$

$$+ \cdots$$

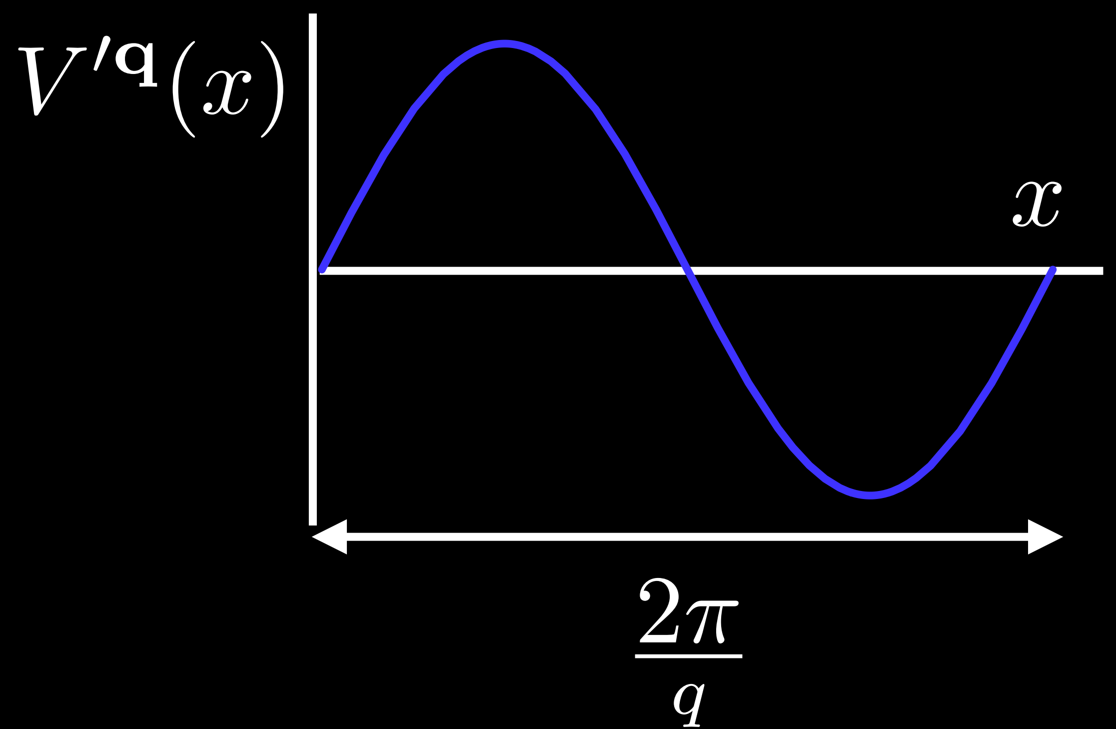
$$\det \left[\frac{\partial^2 E}{\partial \mathbf{u}(\mathbf{R}) \partial \mathbf{u}(\mathbf{R}')} - \omega^2 M(\mathbf{R}) \delta_{\mathbf{R},\mathbf{R}'} \right] = 0$$

monochromatic perturbations



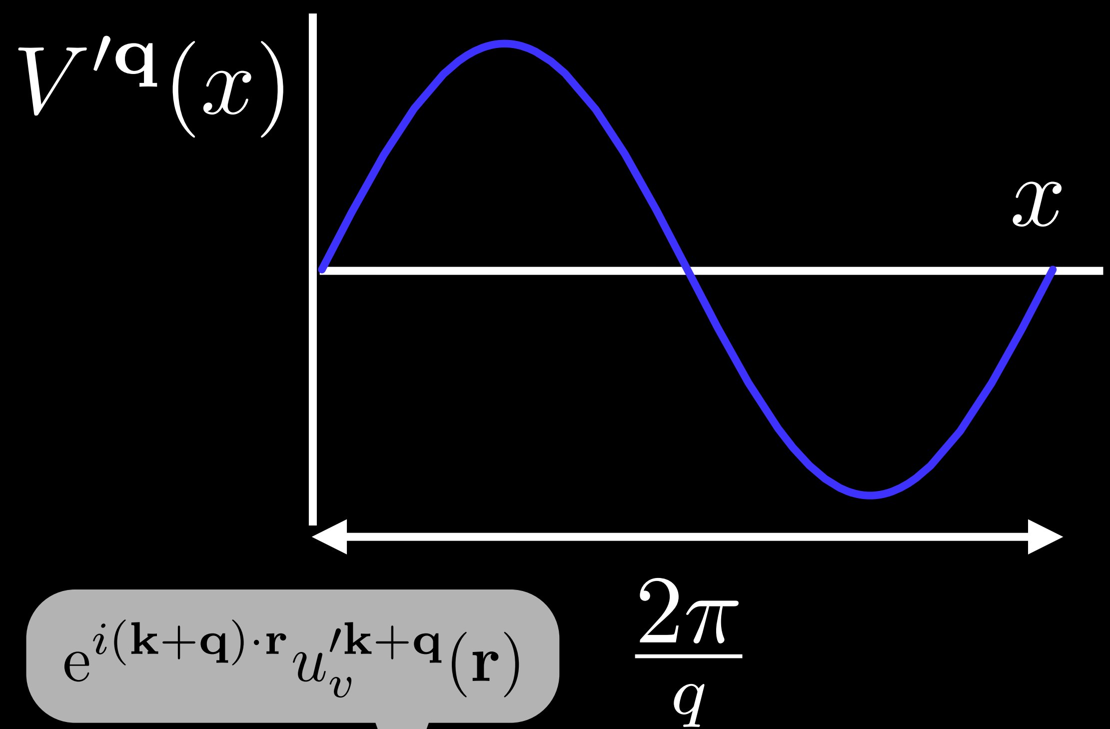
DFPT rhs: $-P_c V'^{\mathbf{q}}_{SCF} \phi^{\mathbf{k}}_v(\mathbf{r})$

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

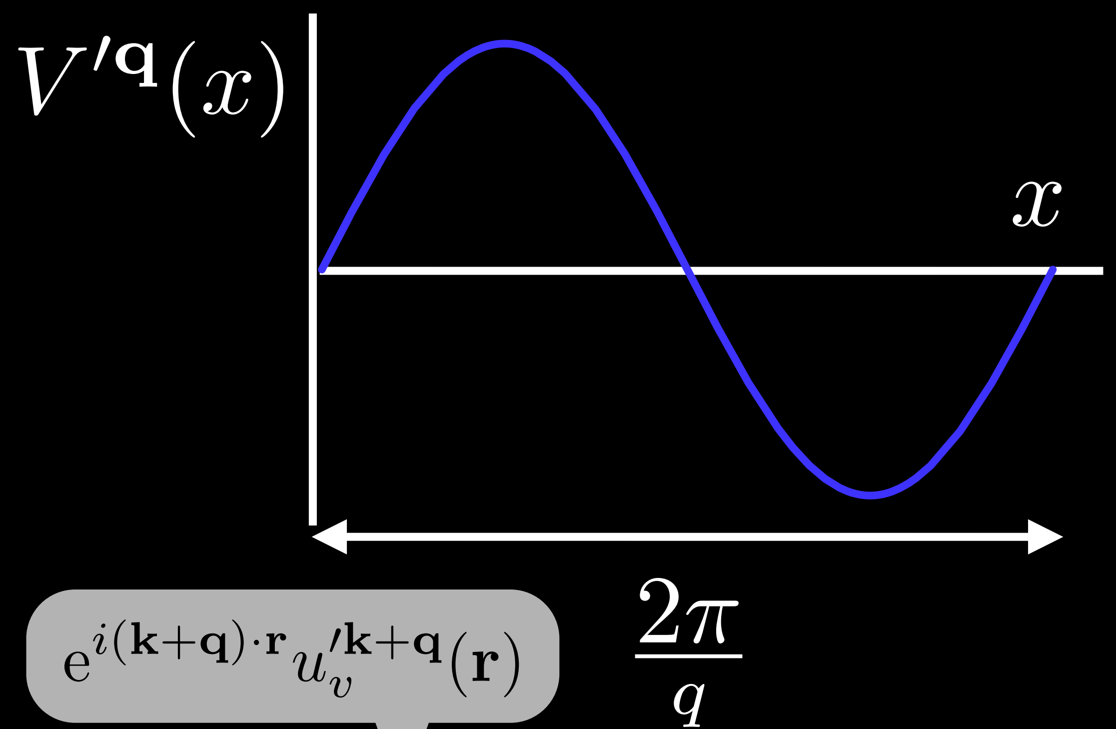


$\mathrm{e}^{i(\mathbf{k}+\mathbf{q})\cdot\mathbf{r}} u_v'^{\mathbf{k}+\mathbf{q}}(\mathbf{r})$

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

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

monochromatic perturbations

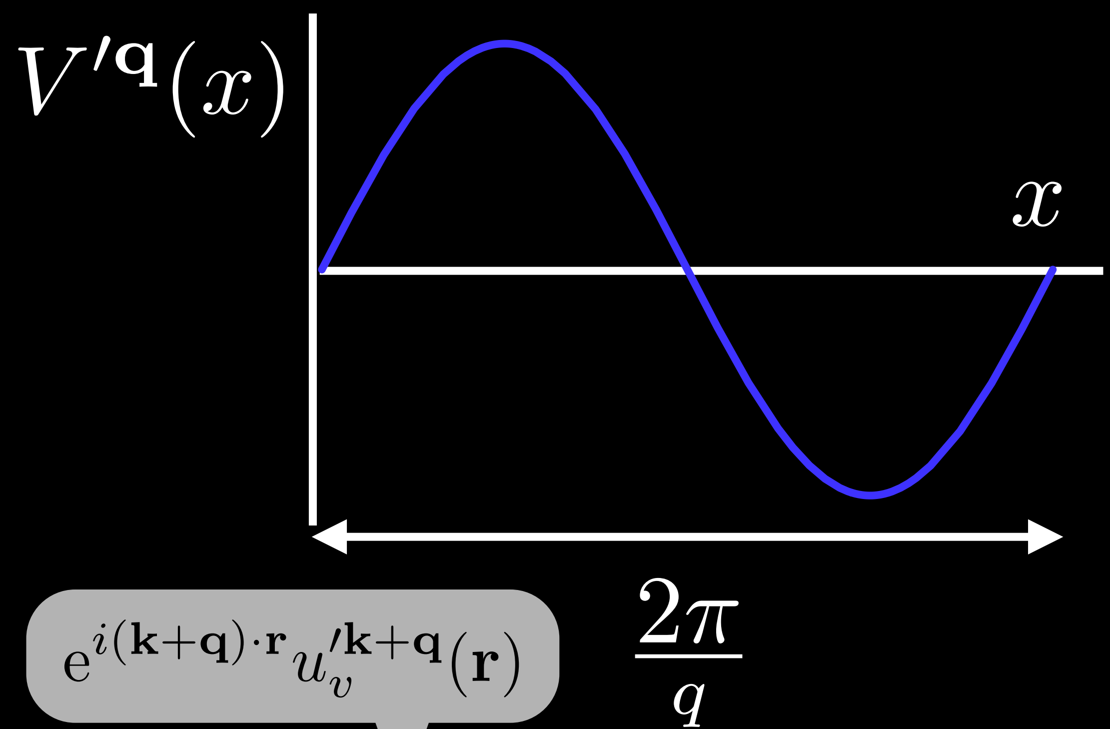


$\mathrm{e}^{i(\mathbf{k}+\mathbf{q})\cdot\mathbf{r}} u_v'^{\mathbf{k}+\mathbf{q}}(\mathbf{r})$ $\qquad$ $\mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}} u_v^{\circ\mathbf{k}}(\mathbf{r})$

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

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

monochromatic perturbations



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

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

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

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

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

phonons in polar materials

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

phonons in polar materials

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

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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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(T)

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$$\mathbf{F}_T = -M\omega_0^2\mathbf{u}$$

phonons in polar materials

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$$\mathrm{div}\ \mathsf{D} \sim i\mathbf{q}\cdot\mathsf{D} = 0$$

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phonons in polar materials

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

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phonons in polar materials

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

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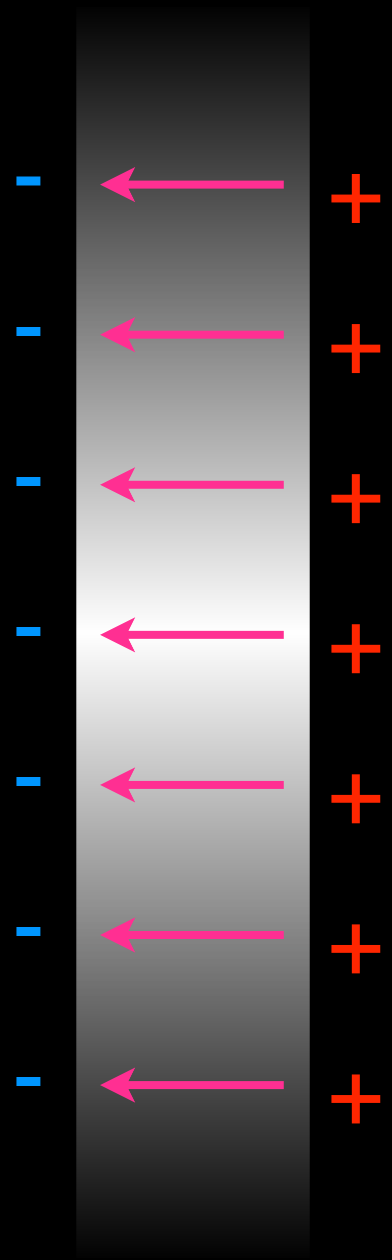
$\mathbf{F}_T = -M\omega_0^2\mathbf{u}$ $\qquad$ $\mathbf{F}_L = -M\left(\omega_0^2 + \frac{4\pi Z^*}{M\Omega\epsilon_\infty}\right)\mathbf{u}$

macroscopic electric fields

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



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

macroscopic electric fields

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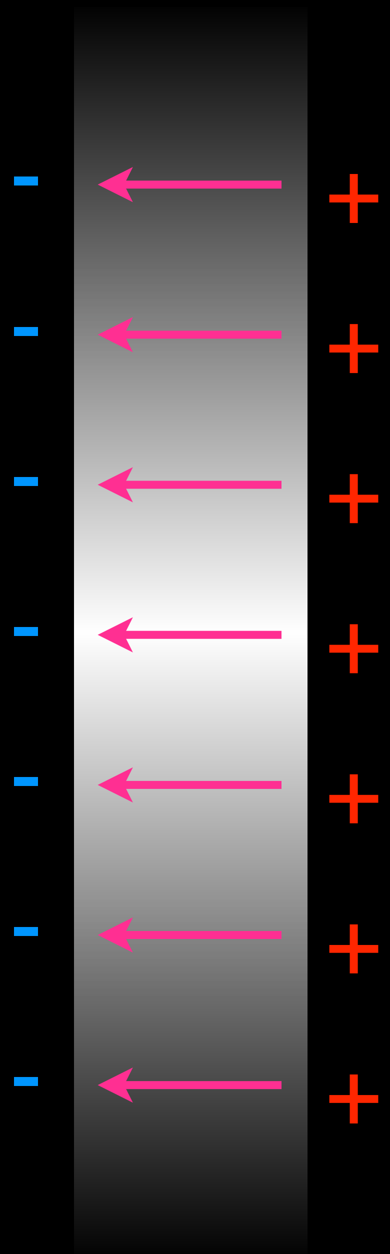

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$$\phi_v^0(\mathbf{r}) \quad = \quad \mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}} u_{v,\mathbf{k}}(\mathbf{r})$$

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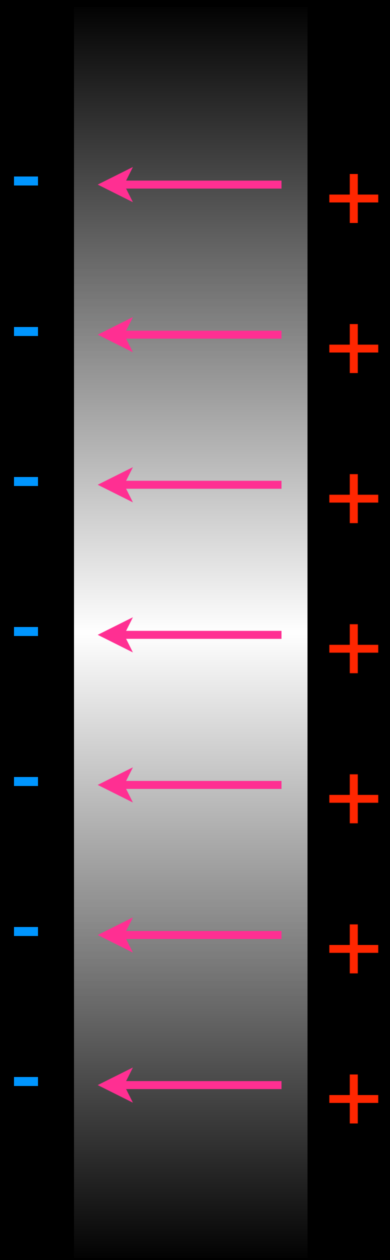

$V'(\mathbf{r}) = \mathbf{E} \cdot \mathbf{r}$

$$\begin{aligned} \phi_v^0(\mathbf{r}) &= \mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}} u_{v,\mathbf{k}}(\mathbf{r}) \\ V'(\mathbf{r})\phi_v^0(\mathbf{r}) &= ?? \end{aligned}$$

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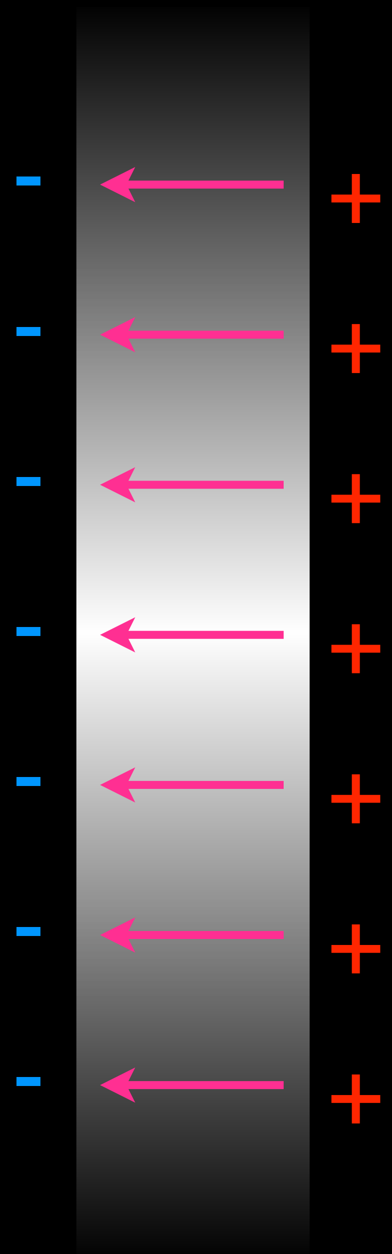

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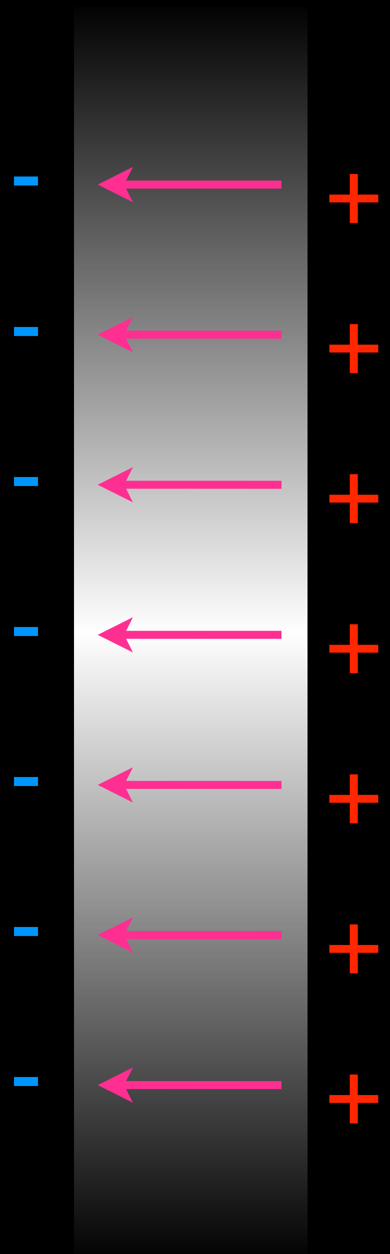

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$$
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V'(\mathbf{r})\phi_v^0(\mathbf{r}) &= ??
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$$

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

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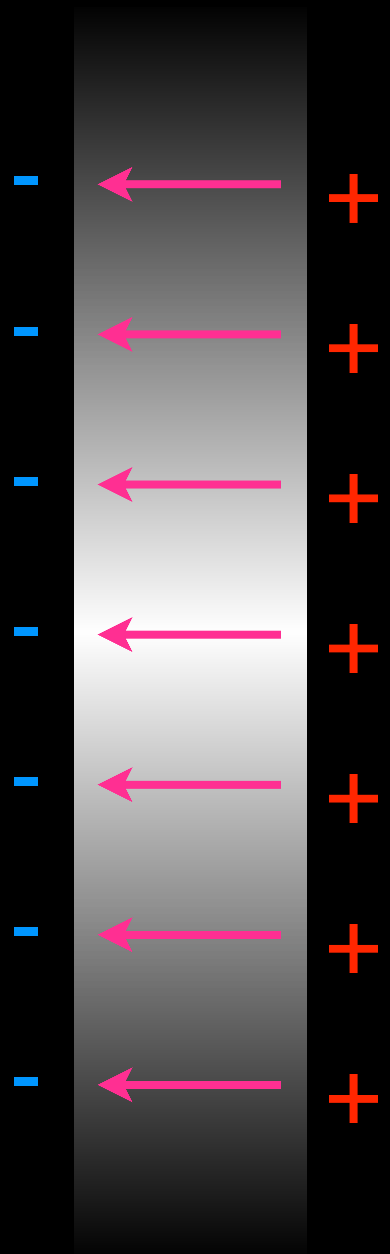

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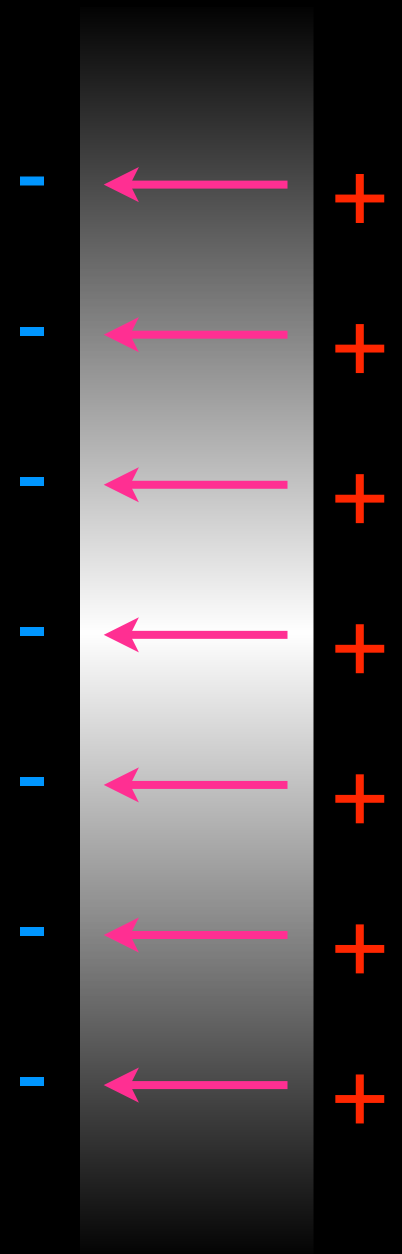
macroscopic electric fields

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



$$\phi_v^0(\mathbf{r}) = \mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}} u_{v,\mathbf{k}}(\mathbf{r})$$
$$V'(\mathbf{r})\phi_v^0(\mathbf{r}) = ??$$

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

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

DFPT rhs

interatomic force constants

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

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short ranged +
dipole-dipole

interatomic force constants

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short ranged +
dipole-dipole

- remove the 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 you may need for practical purposes (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-periodic perturbations: OK

DFPT: the main features

- response functions calculated in terms of response orbitals, $\{\phi'_v\}$
- solve the linear system: $\phi_v \mapsto H_{KS}\phi_v$; do not calculate empty (conduction) states
- calculate the response to the perturbation you want, only
- non-local perturbations: OK
- non-periodic perturbations: OK
- macroscopic electric fields: OK

VOLUME 62, NUMBER 24 PHYSICAL REVIEW LETTERS 12 JUNE 1989

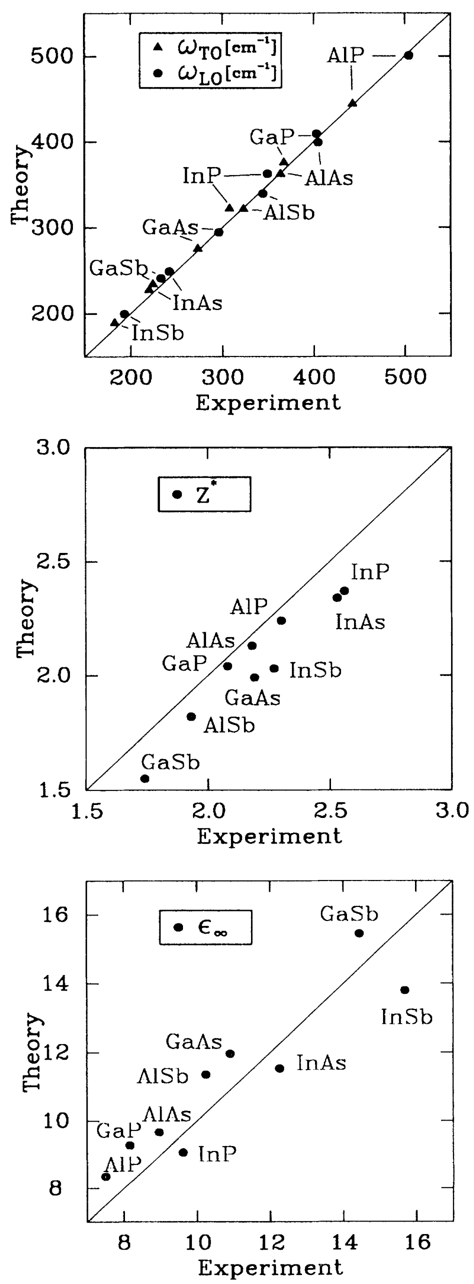
Piezoelectric Properties of III-V Semiconductors from First-Principles Linear-Response Theory

Stefano de Gironcoli[(a)]
Dipartimento di Fisica Teorica, Università di Trieste, Strada Costiera 11, I-34014 Trieste, Italy

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

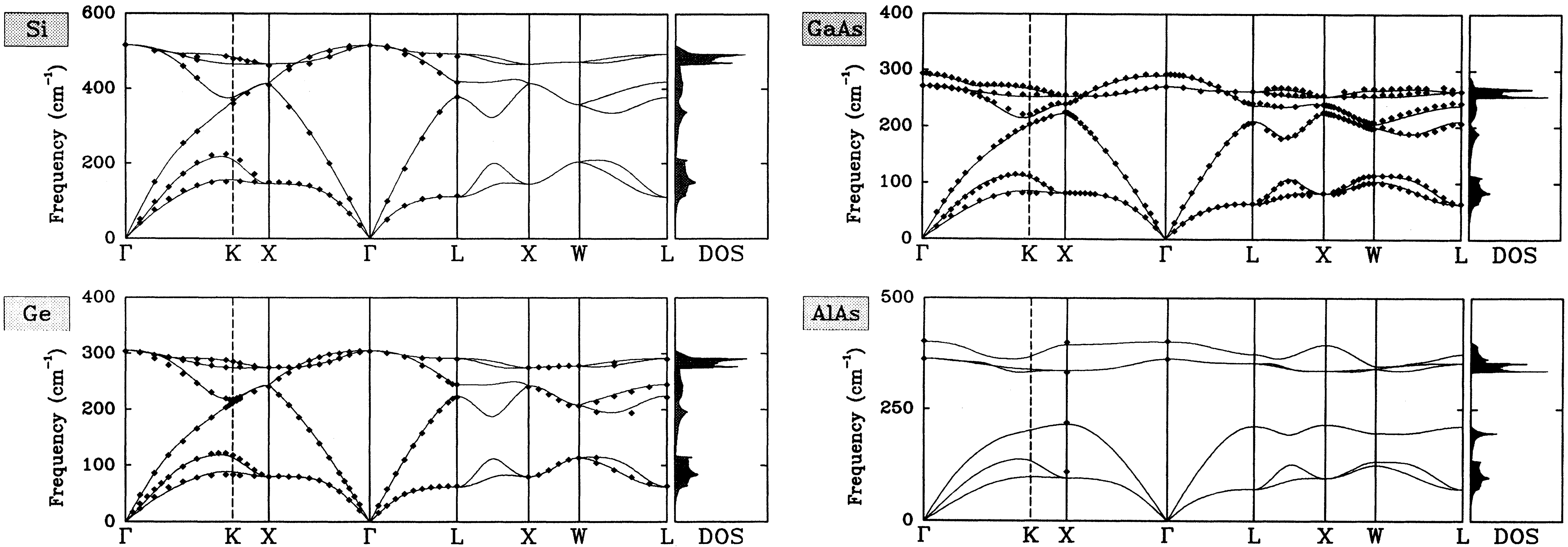
Raffaele Resta[(b)]
Institut Romand de Recherche Numérique en Physique des Matériaux (IRRMA), Ecole Polytechnique Fédérale de Lausanne, CH-1015, Lausanne, Switzerland

(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)

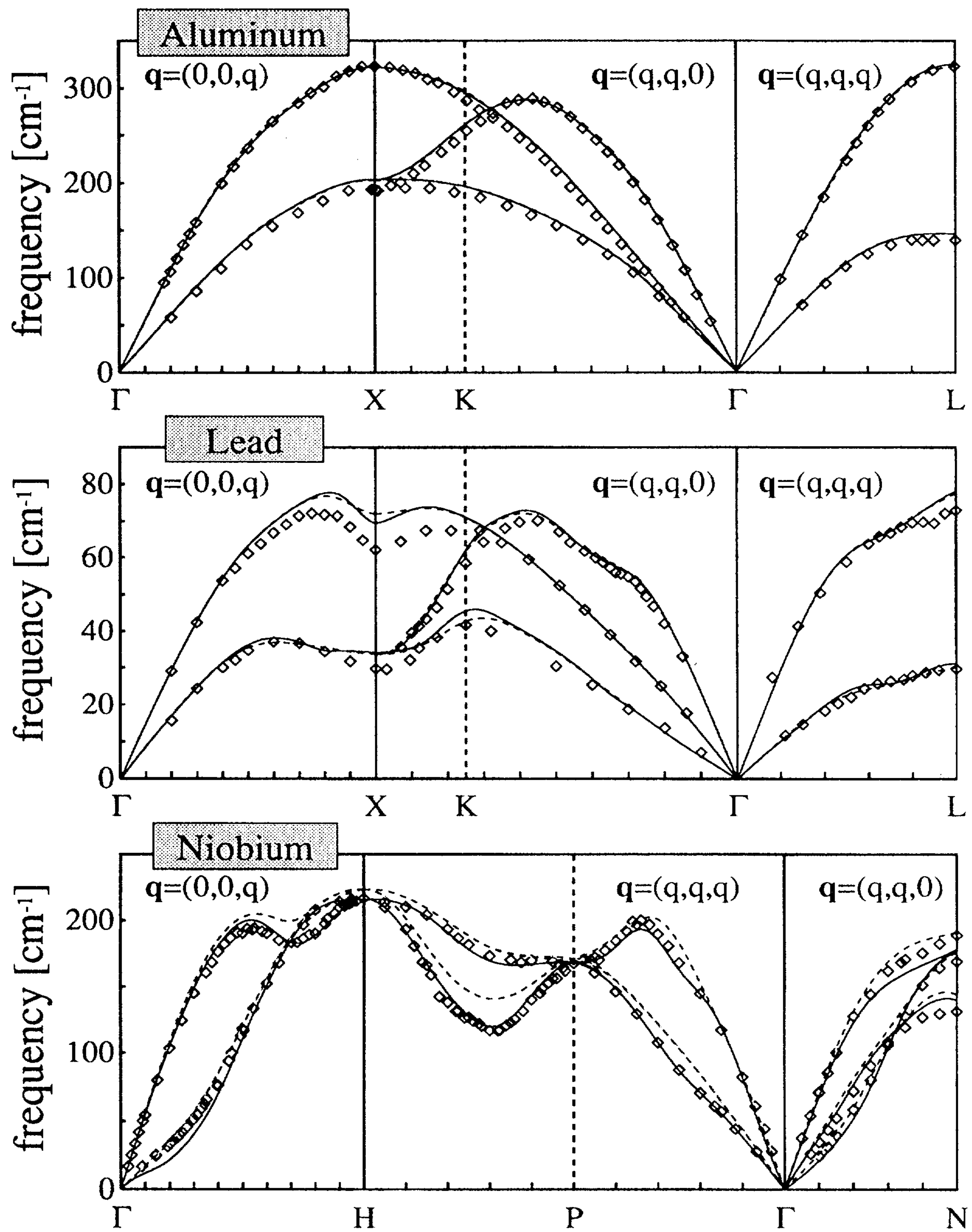
phonons from DFPT



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

MA PER SEGUIR VIRTUTE E CANOSCENZA

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
- …

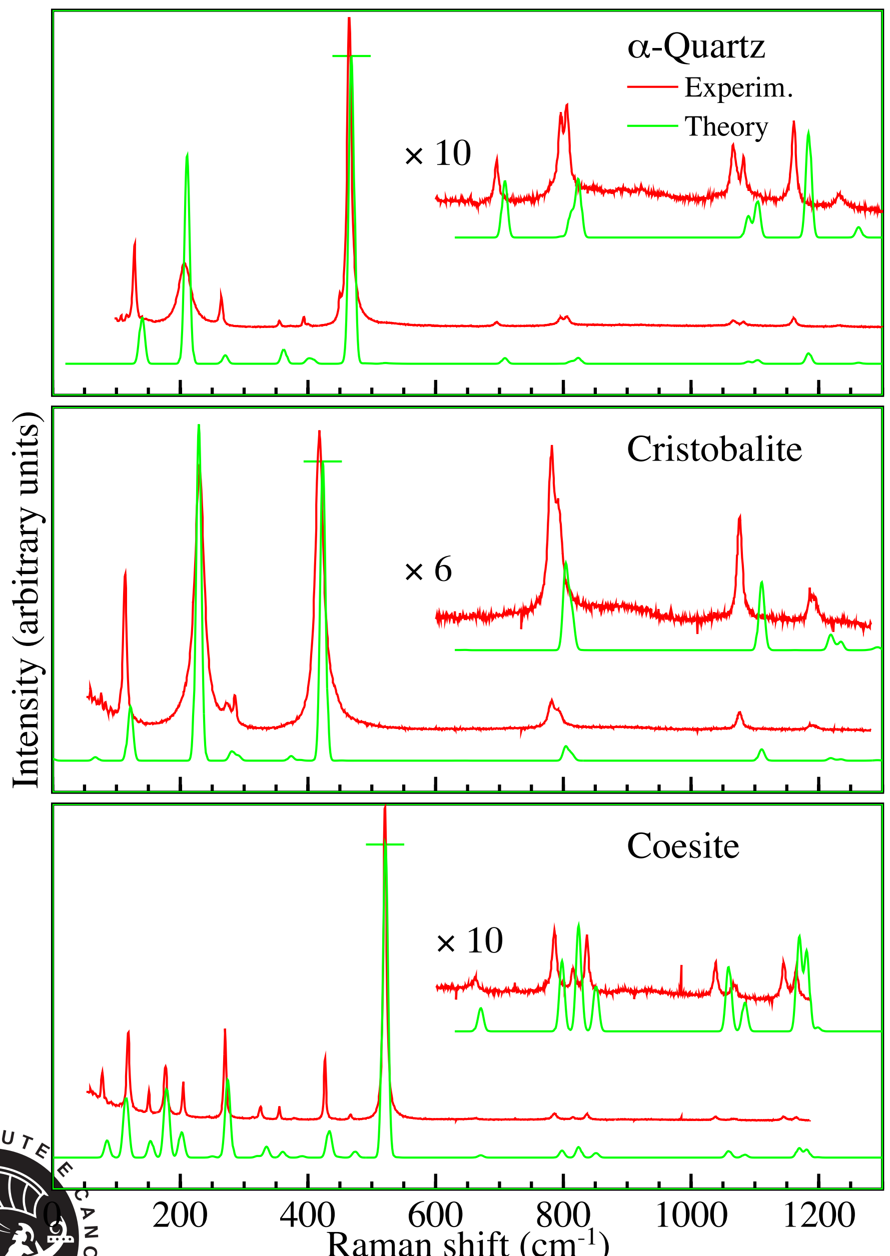
SB, A. Dal Corso, S. de Gironcoli, and P. Giannozzi, *Phonons and related crystal properties from density-functional perturbation theory*, Rev. Mod. Phys. **73**, 515 (2001)

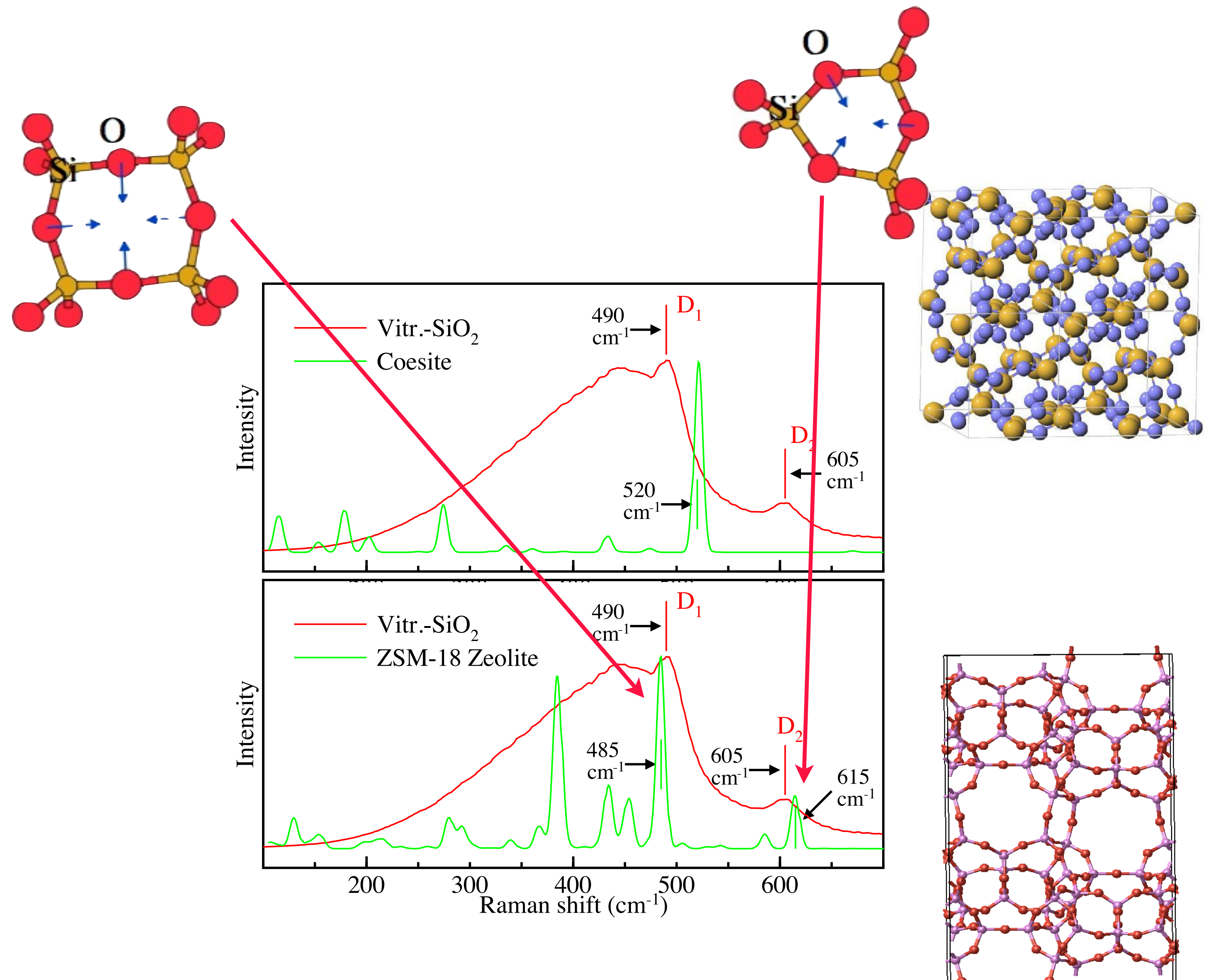
a sampler of more recent applications

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





a sampler of recent applications

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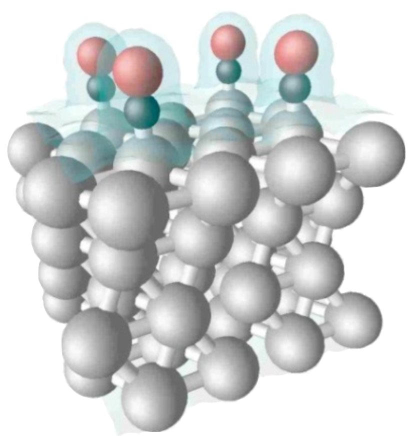
ARTICLES
Published on Web 08/17/2007

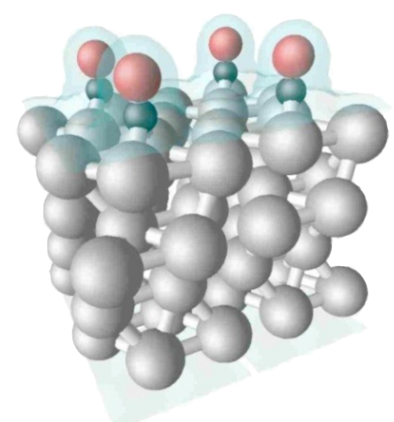
Vibrational Recognition of Adsorption Sites for CO on Platinum and Platinum−Ruthenium Surfaces

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

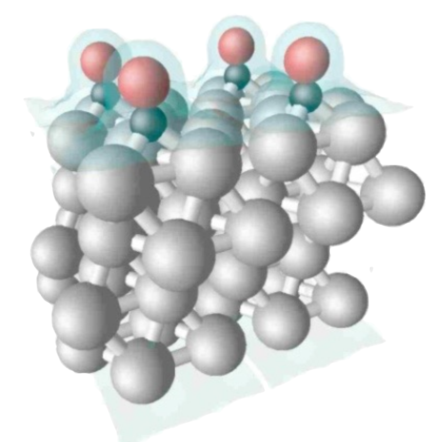
11046 J. AM. CHEM. SOC. ■ VOL. 129, NO. 36, 2007



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

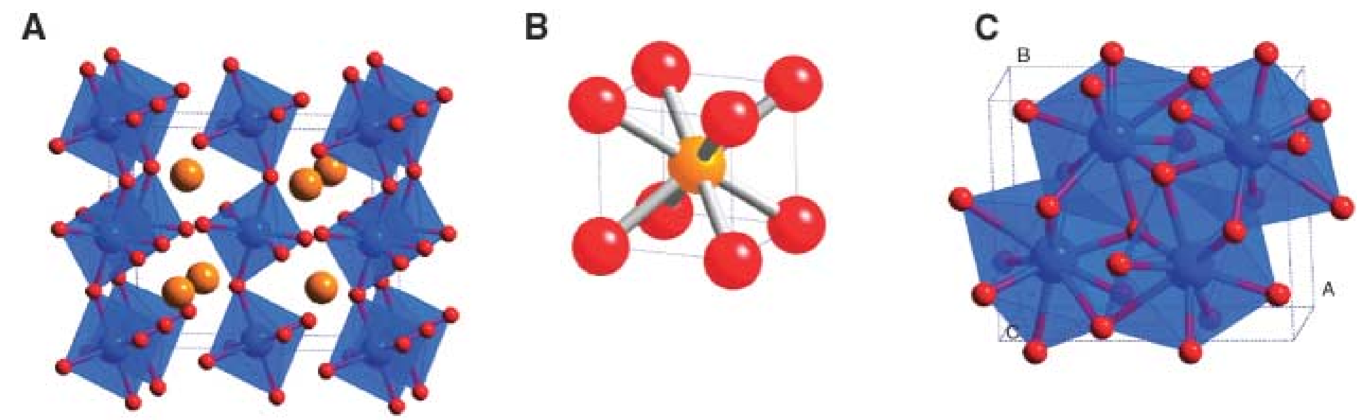
DFT

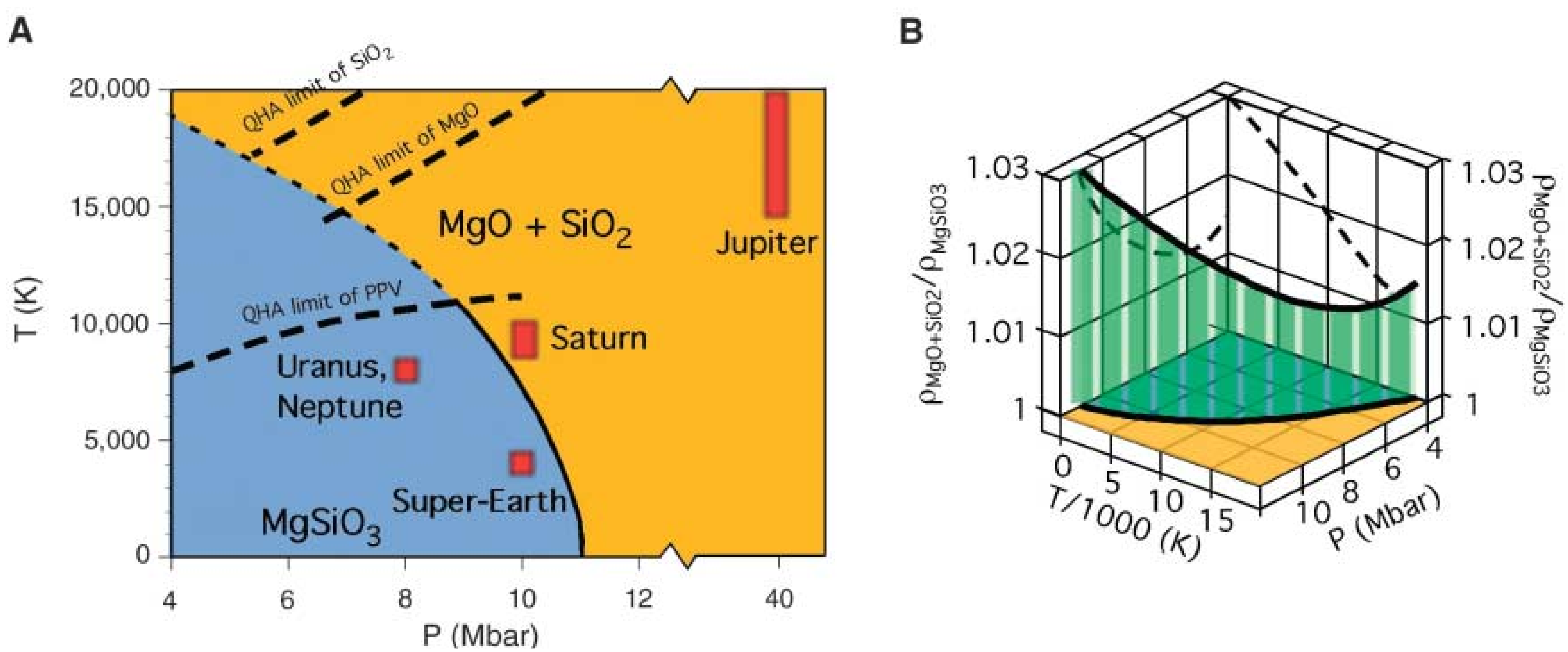
a sampler of recent applications

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





a sampler of recent applications

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

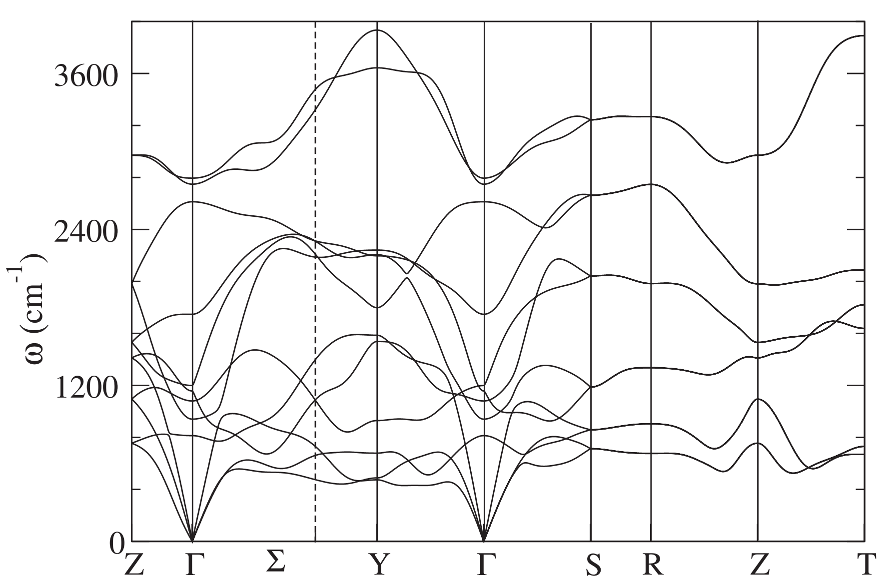
Ab Initio Description of High-Temperature Superconductivity in Dense Molecular Hydrogen

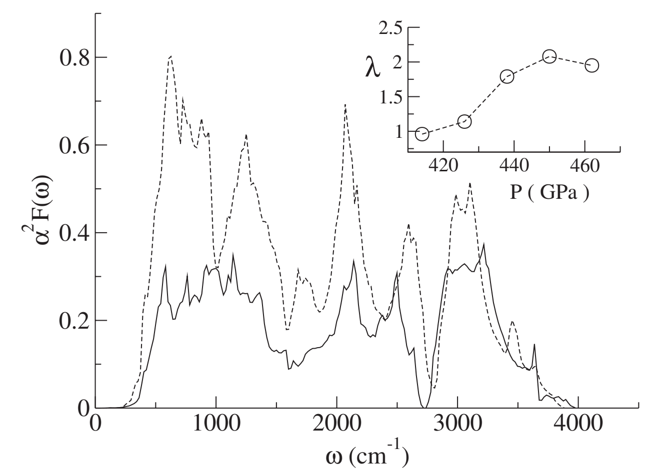
P. Cudazzo,[1] G. Profeta,[1] A. Sanna,[2,3] A. Floris,[3] A. Continenza,[1] S. Massidda,[2] and E. K. U. Gross[3]

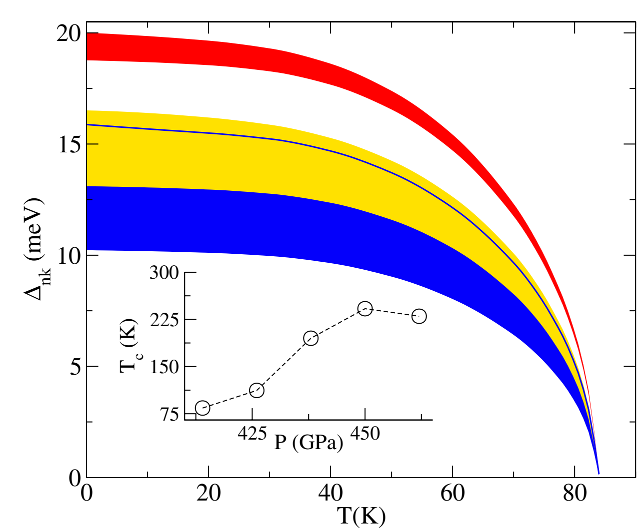
[1]*CNISM - Dipartimento di Fisica, Università degli Studi dell'Aquila, Via Vetoio 10, I-67010 Coppito (L'Aquila) Italy*
[2]*SLACS-INFM/CNR—Dipartimento di Fisica, Università degli Studi di Cagliari, I-09124 Monserrato (CA), Italy*
[3]*Institut für Theoretische Physik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin, Germany*

(Received 7 December 2007; published 23 June 2008; corrected 27 June 2008)

414 GPa







a sampler of recent applications

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*
[3]*Institut für Theoretische Physik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin, Germany*

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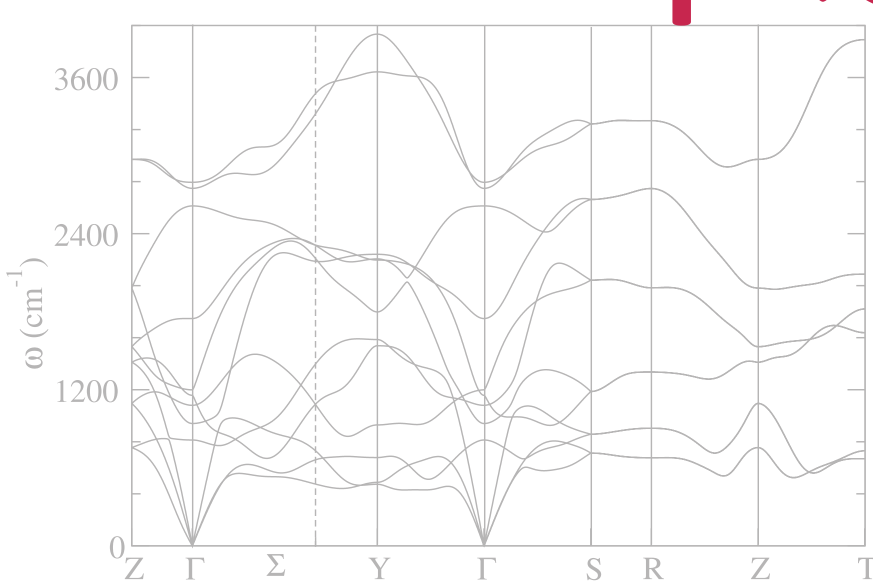
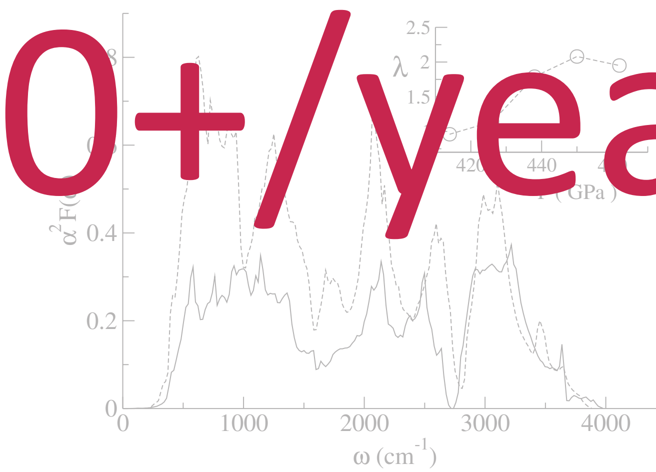
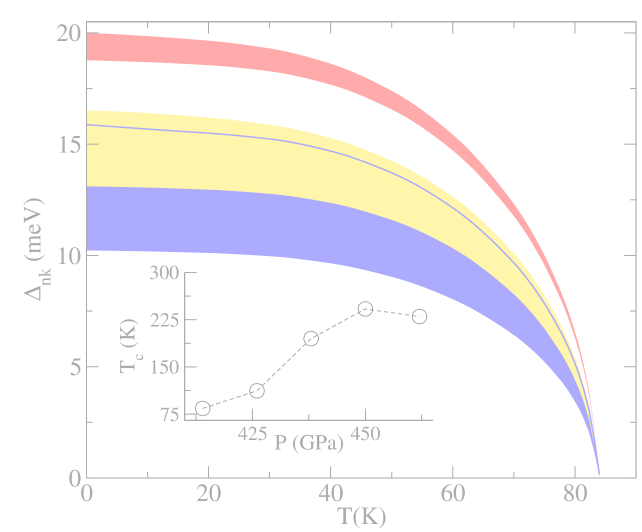
• • • + ≈600+/year

414 GPa







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these slides shortly at
http://talks.baroni.me