SELECTION RULES FOR INTERSUBBAND TRANSITIONS IN VALLEY SPLIT [001]-SiGe QUANTUM WELLS

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NATIONAL ENTERPRISE FOR NANOSCIENCE AND NANOTECHNOLOGY

NEST-INFM-CNR

Università di Pisa

Outline

- Intervalley interaction in confined [001]-SiGe structures
- Tight-binding description of SiGe multilayers
- Valley splitting oscillation
- Selection rules and signature of intervalley interaction in the intersubband absoption
- Conclusions

Experimental

- A. B. Fowler et al., Phys. Rev. Lett. **16,** 901 (1966).
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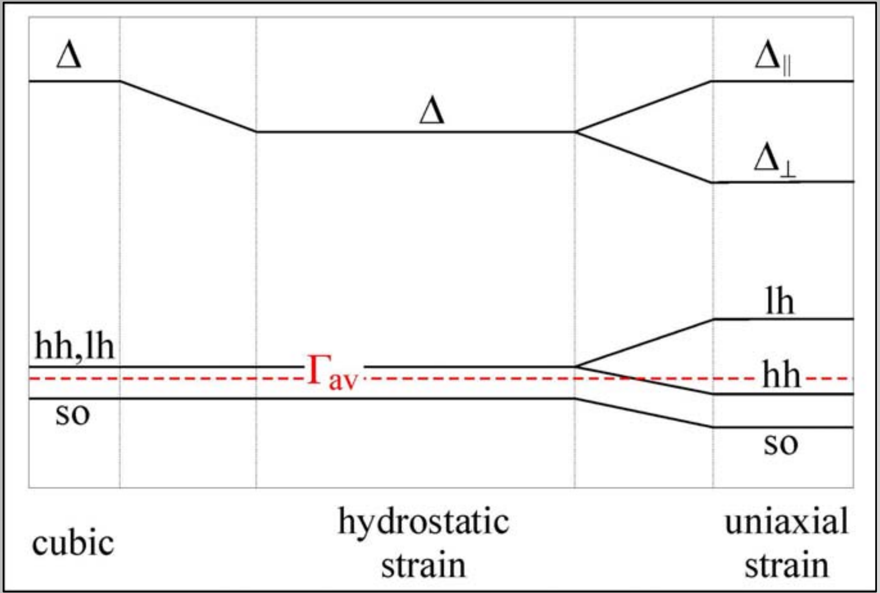
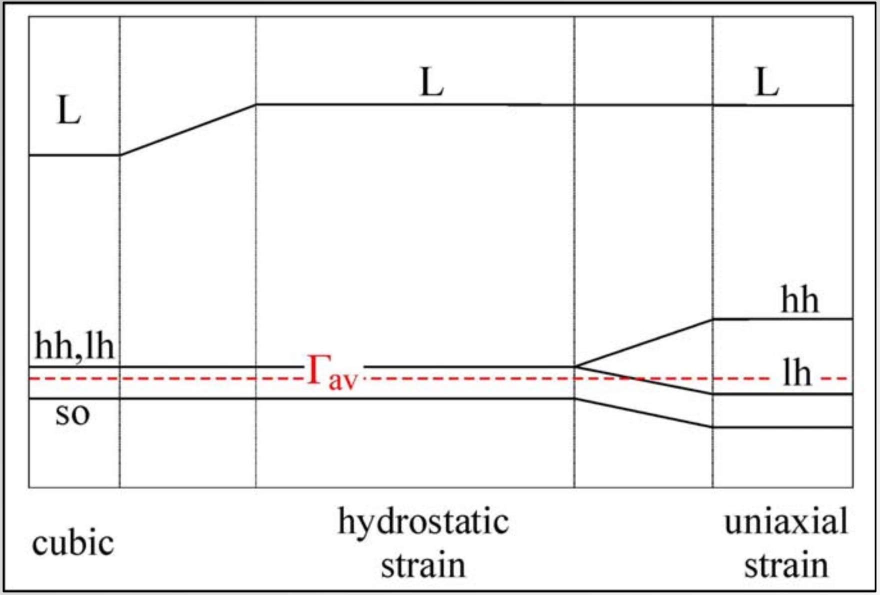
- K. Takashina et al., Phys. Rev. Lett. **96,** 236801 (2006).
- M. A. Wilde et al. Phys. Rev. B **72,** 165429 (2005).

Theoretical

- L. J. Sham and M.Nakayama, Phys. Rev. B **20** 734 (1979).
- ....
- T. B. Boykin et al., Appl. Phys. Lett. **84,** 115 (2004).
- M. O. Nestoklon, L. E. Golub, and E. L. ivchenko Phys. Rev. B **73,** 235334 (2006).
- A. Valavanis, Z. Ikonić, and R. W. Kelsall, Phys. Rev. B **75,** 205332 (2007).



Δ
Δ
$\Delta_{\|}$
$\Delta_{\perp}$
lh
hh,lh
Γ_{av}
hh
so
so
cubic
hydrostatic
strain
uniaxial
strain



L
L
L
hh
hh,lh
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lh
so
cubic
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uniaxial
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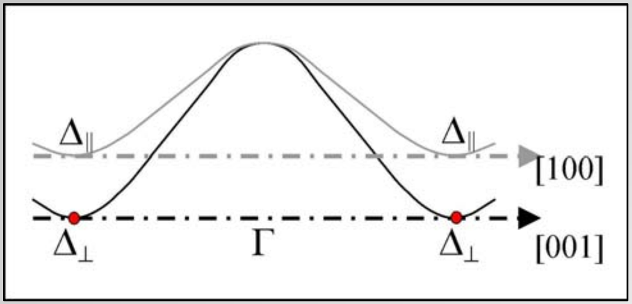
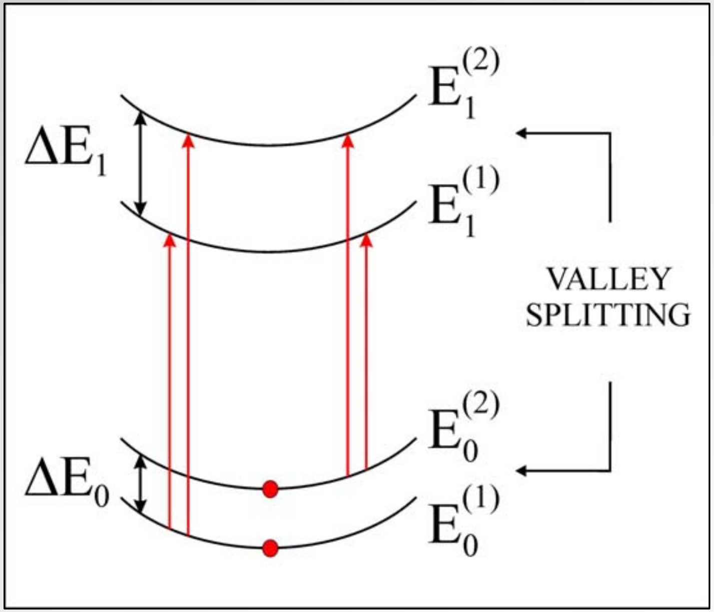
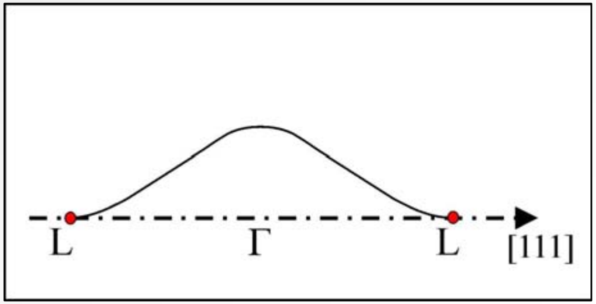


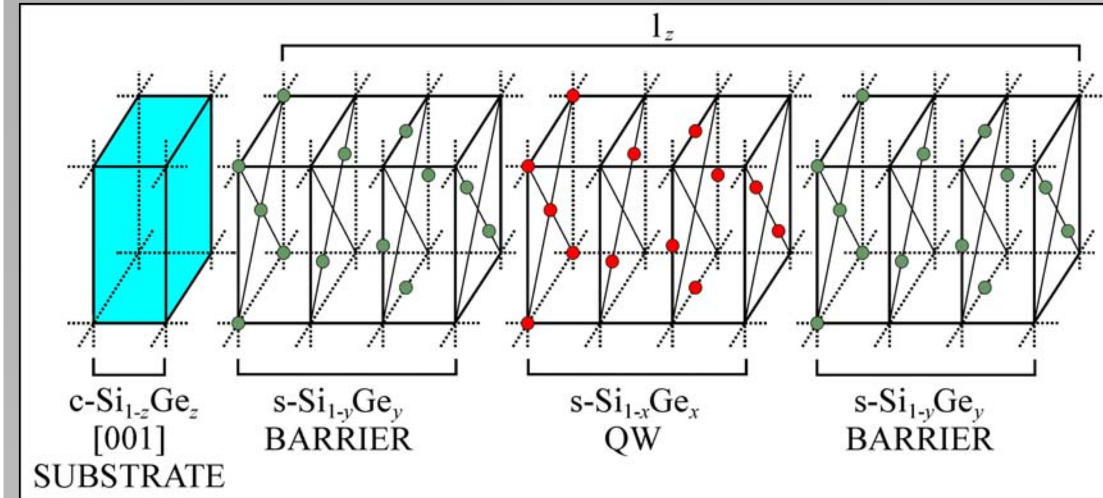
$\Delta_{\|}$
$\Delta_{\|}$
[100]
$\Delta_{\perp}$
Γ
$\Delta_{\perp}$
[001]

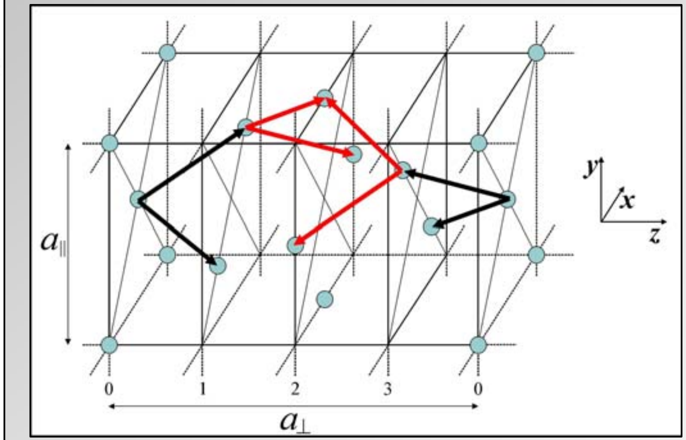


$E_1^{(2)}$
ΔE_1
$E_1^{(1)}$
VALLEY
SPLITTING
$E_0^{(2)}$
ΔE_0
$E_0^{(1)}$

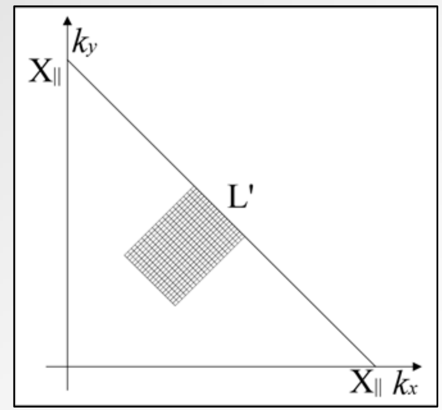


L
Γ
L
[111]





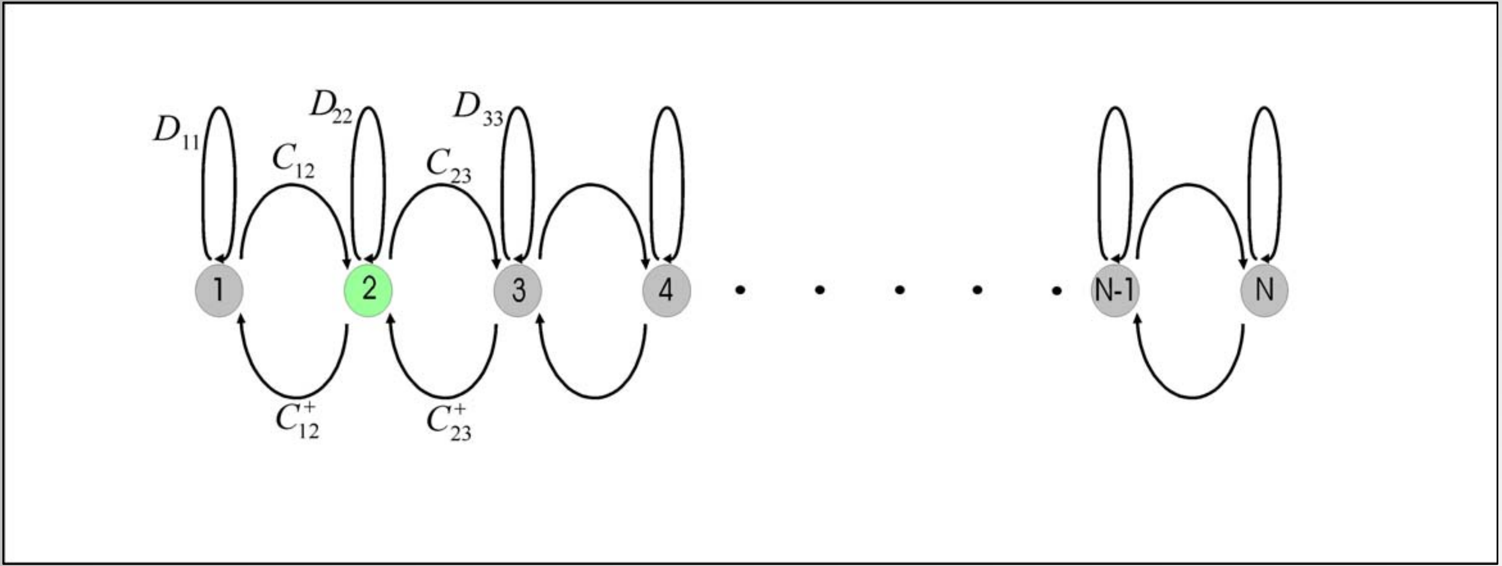
- Macroscopic **ELASTICITY THEORY** for the atomic site positions
- ***s,p,d*** and ***s**** orbital with **SPIN-ORBIT** coupling and **FIRST-NEIGHBOR** interaction.
- Self and hopping energies reproduce **BULK Si** and **Ge** band structure.
- **VIRTUAL CRYSTAL APPROXIMATION** for **SiGe** alloys.

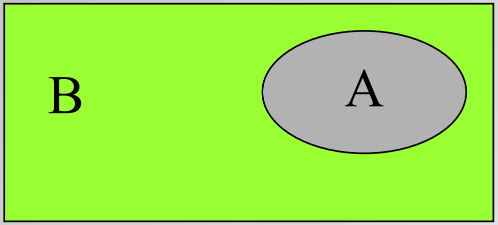


$$\langle \Psi^f(\vec{k},\vec{r})|\hat{\epsilon}\cdot\vec{p}|\Psi^i(\vec{k},\vec{r})\rangle = \hat{\epsilon}\cdot\vec{p}^{\,fi}(\vec{k})$$

$$\vec{p}^{\,fi}(\vec{k}) = \sum_{m,l}\sum_{\mu,\nu} A_m^{\mu *}(\vec{k},f)A_l^{\nu}(\vec{k},i)\sum_n e^{ik_z\tau_{nz}} e^{\vec{k}_{\|}\cdot(\vec{\tau}_n+\vec{d}_\nu-\vec{d}_\mu)}\langle\phi_m(\vec{r}-\vec{d}_\mu)|\vec{p}|\phi_l(\vec{r}-\vec{\tau}_n-\vec{d}_\nu)\rangle$$

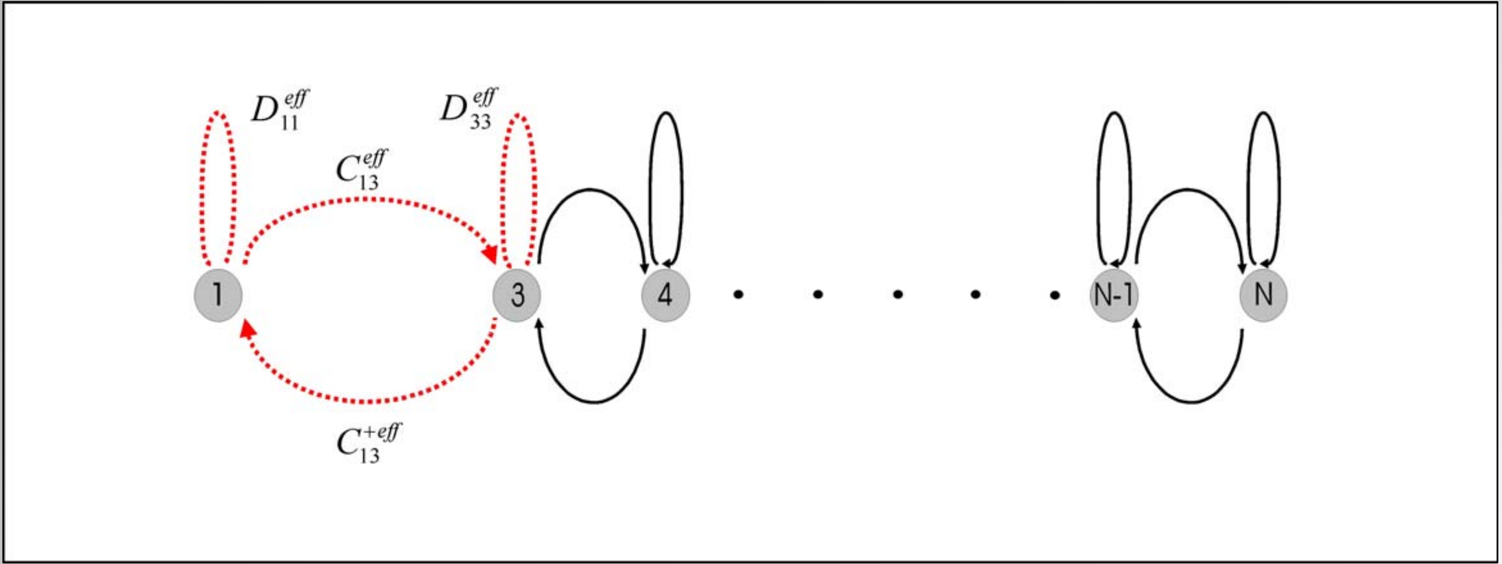
Decimation-renormalization method

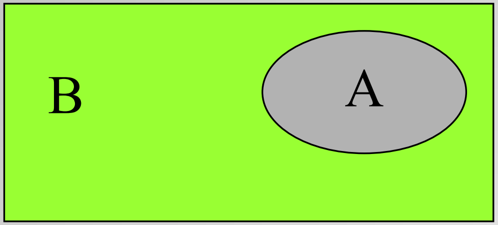




$$G_{AA} = \frac{1}{E - H_{AA} - H_{AB}\dfrac{1}{E - H_{BB}}H_{BA}}$$

Decimation-renormalization method

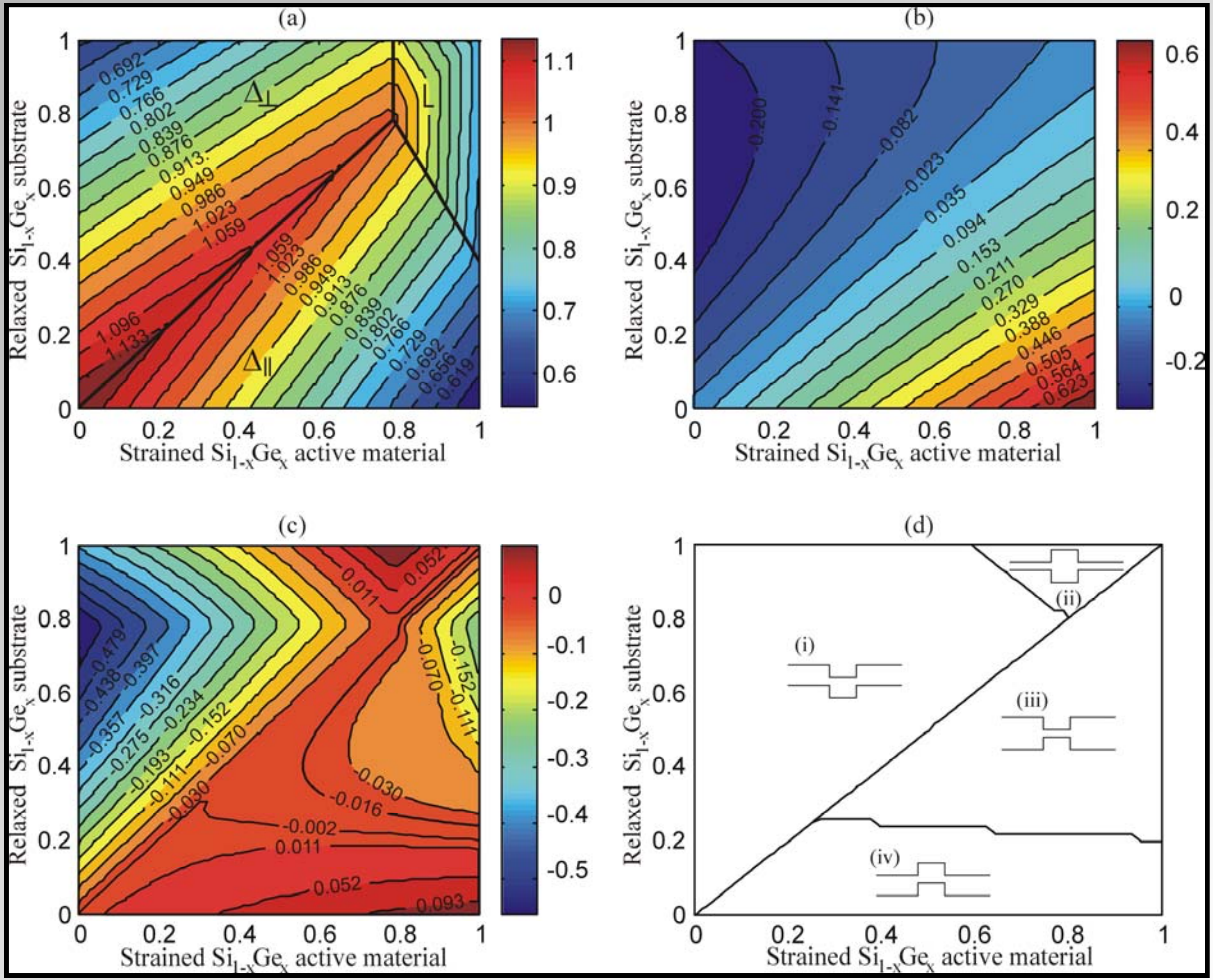




$$G_{AA} = \frac{1}{E - H_{AA} - H_{AB}\dfrac{1}{E - H_{BB}}H_{BA}}$$

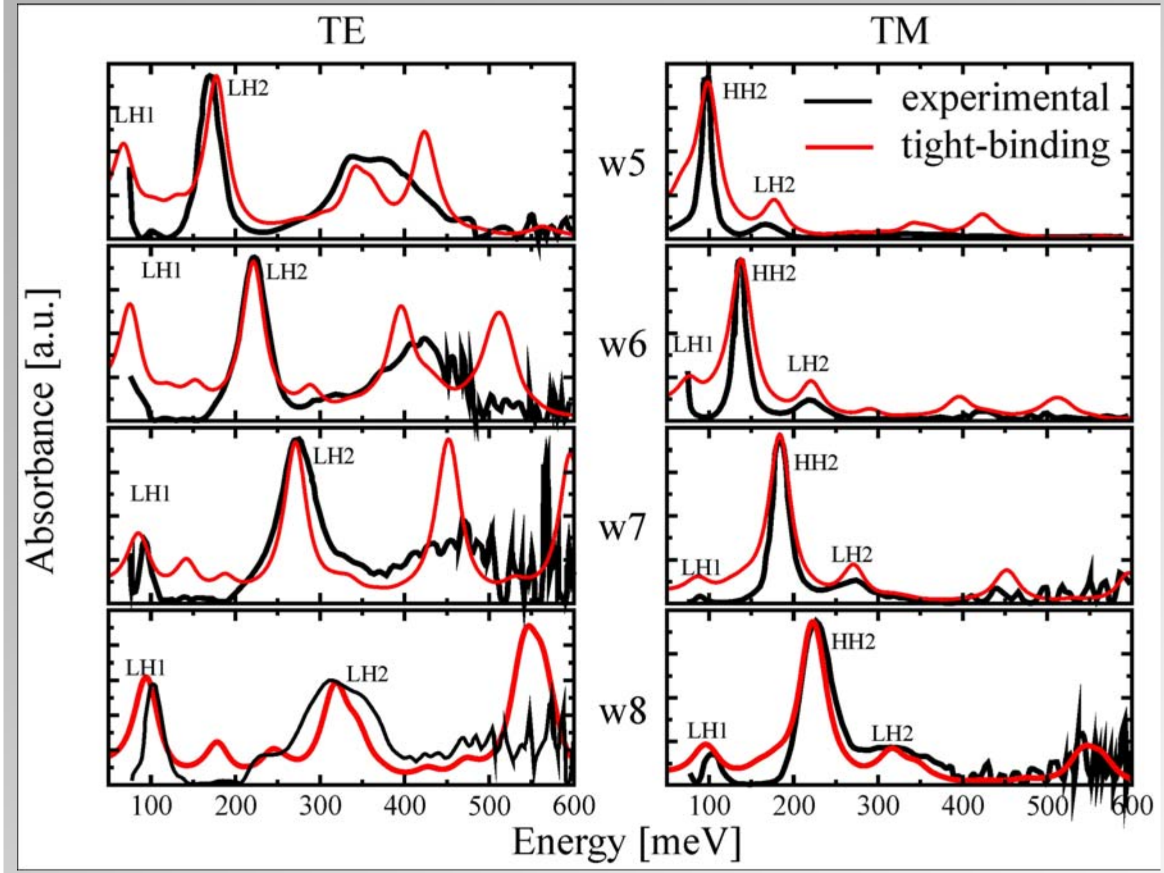
$$\begin{aligned}
D_{1,1}^{(eff)} &= D_{1,1} + C_{1,2}\frac{1}{E - D_{2,2}}C_{1,2}^{\dagger} \\
D_{3,3}^{(eff)} &= D_{3,3} + C_{2,3}^{\dagger}\frac{1}{E - D_{2,2}}C_{2,3} \\
C_{1,3}^{(eff)} &= C_{1,2}\frac{1}{E - D_{2,2}}C_{2,3} \\
C_{3,1}^{(eff)} &= C_{2,3}^{\dagger}\frac{1}{E - D_{2,2}}C_{1,2}^{\dagger}
\end{aligned}$$

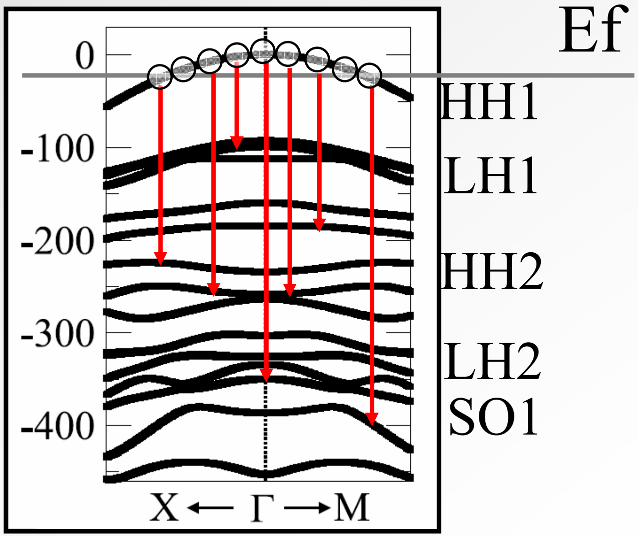
Band edges profiles for Si_yGe_{1-y}/Si_xGe_{1-x} heterointerfaces



M. Virgilio, and G. Grosso, J. of Phys. : Condes. Matter., **18,** 1021 (2006)

Valence intersubband transitions in SiGe QW





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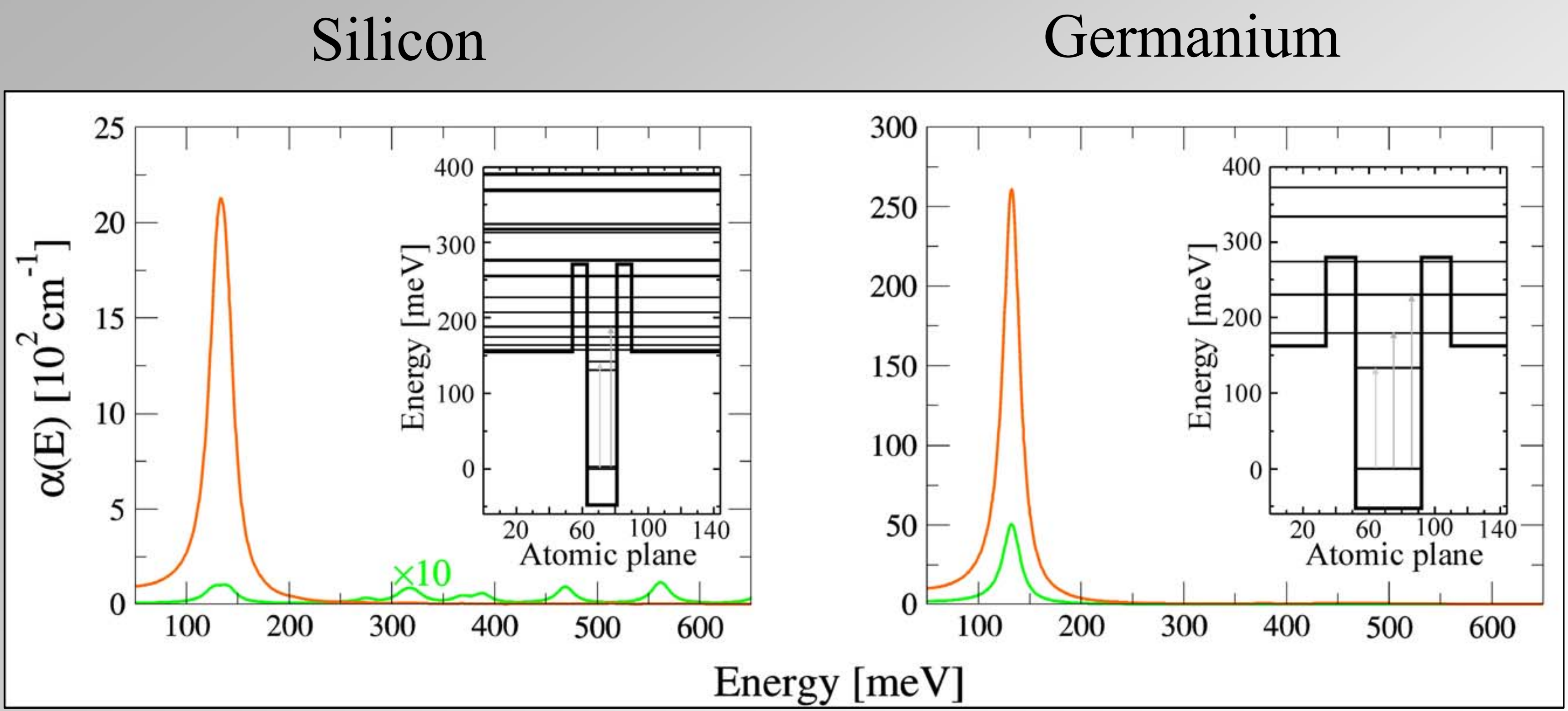
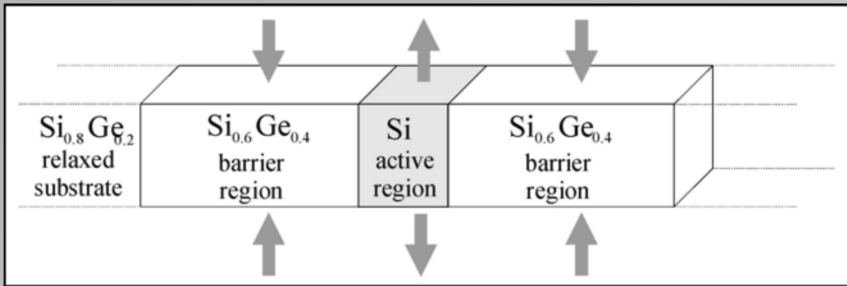
Conduction intersubband absorption at normal incidence

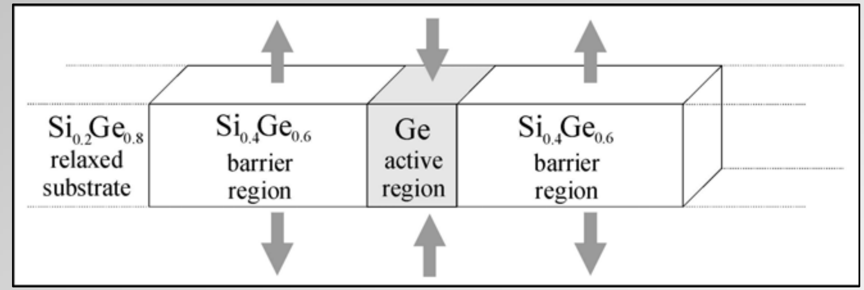


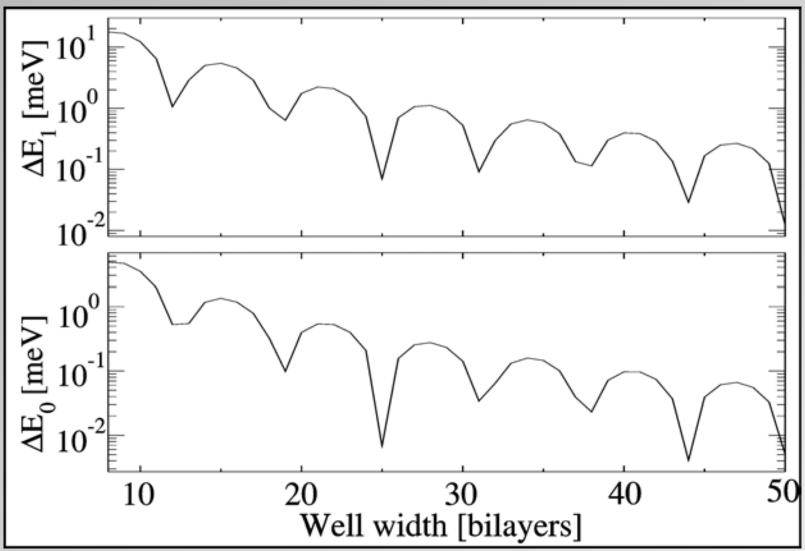
$m_{xz}, m_{yz} = 0$ parallel normal $m_{xz}, m_{yz} \neq 0$

M. Virgilio and G. Grosso, Nanotechnology, **18**, 075402 (2007);

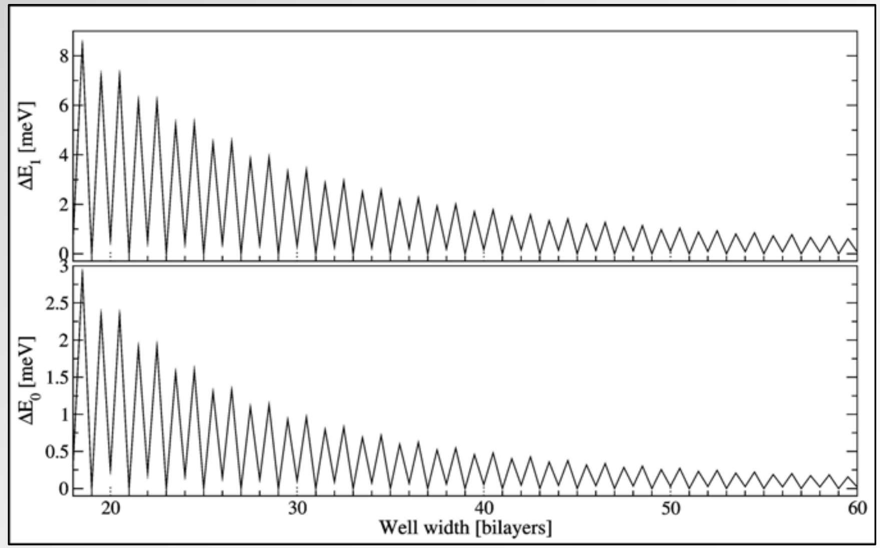
Valley splitting oscillations







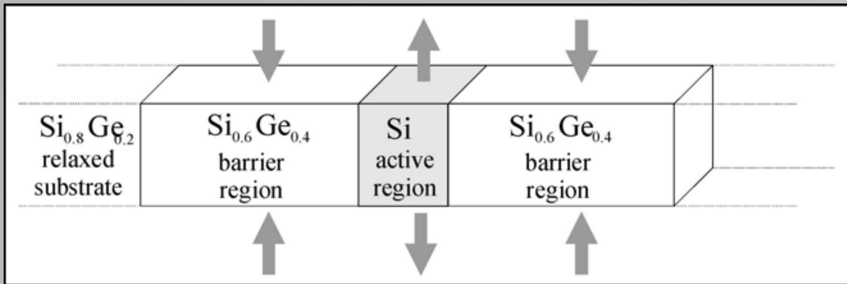
Silicon

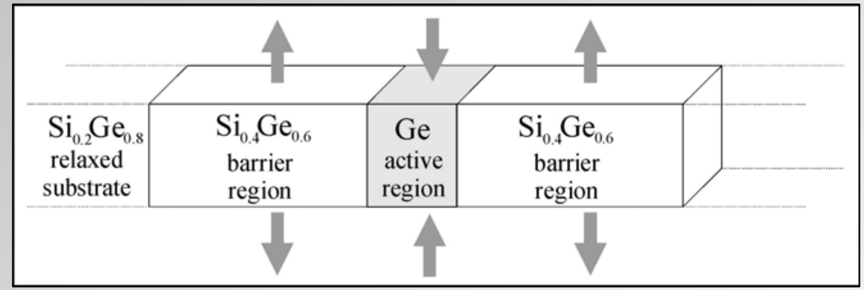


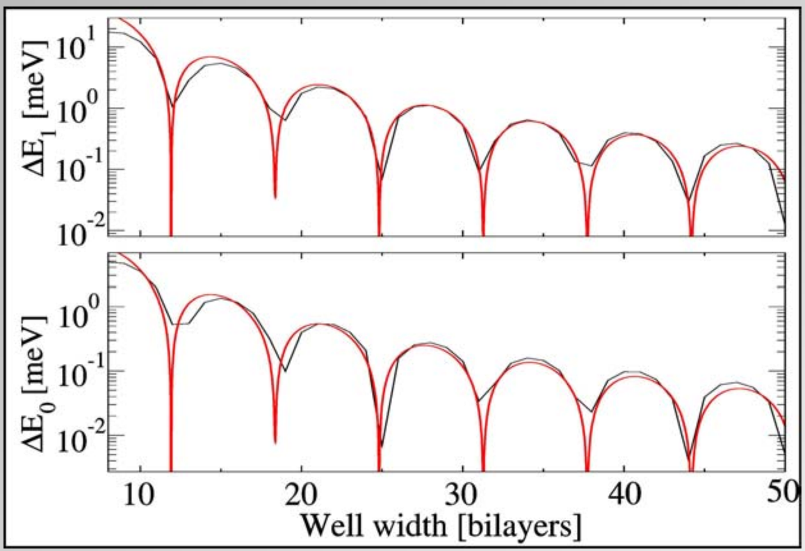
Germanium

$$\Delta E \propto (\zeta + z)^{-3} \sin[(\zeta + z)\phi_{min}]$$

Valley splitting oscillations







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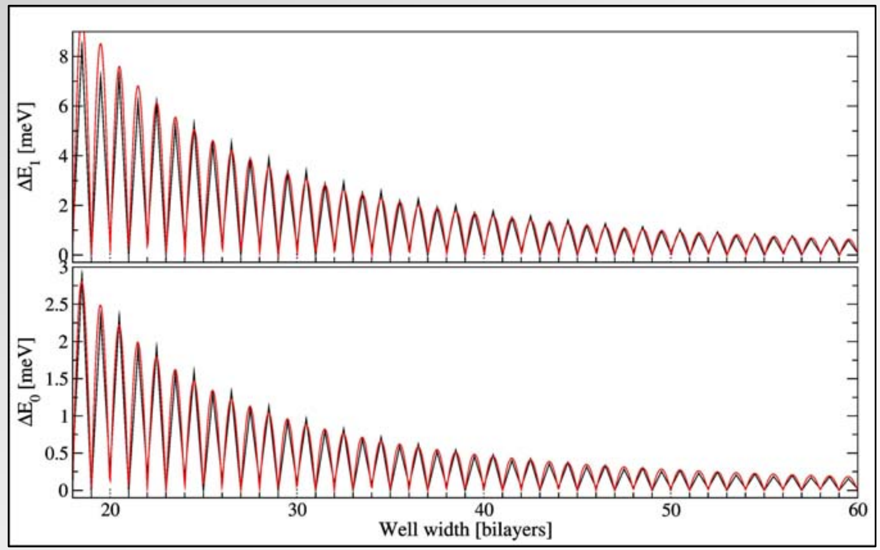
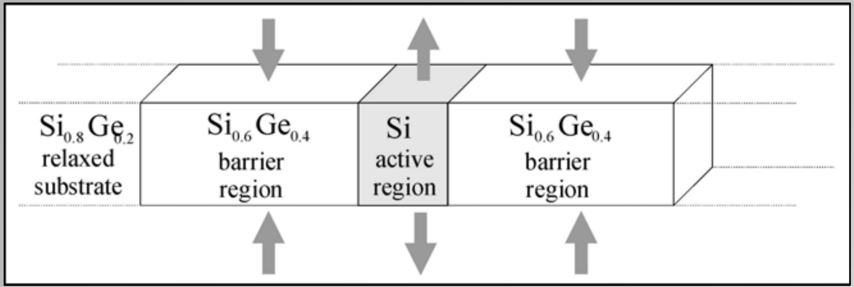
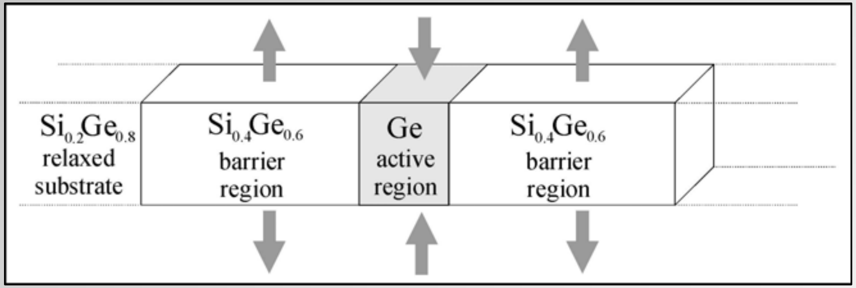


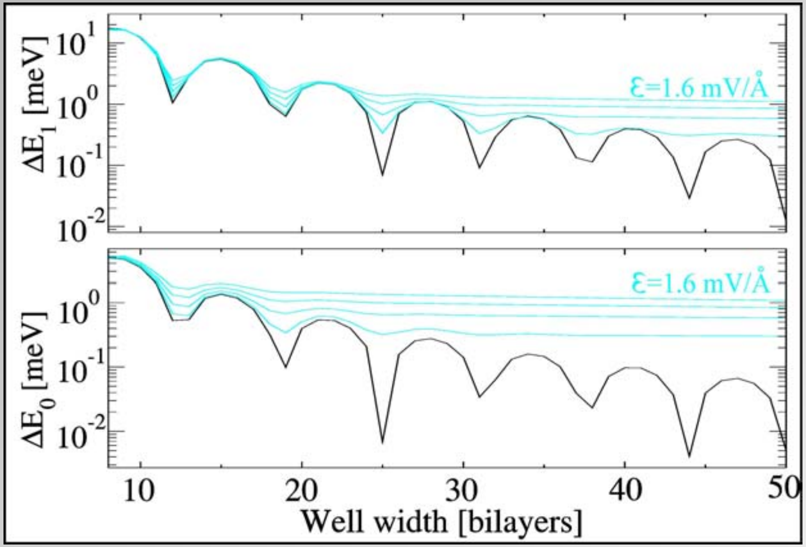
Germanium

$\Delta E = \propto (z+\varsigma)^{-3} \sin[(z+\varsigma)\phi_{min}]$

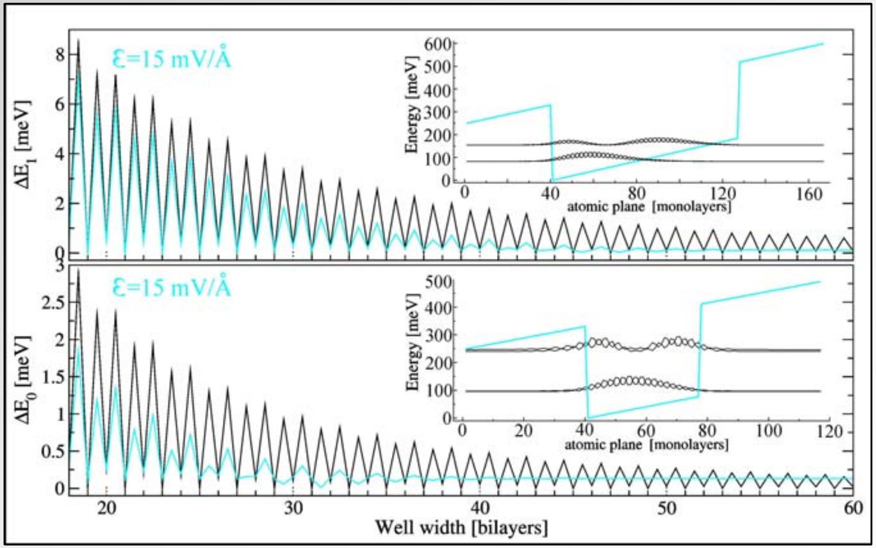
Valley splitting oscillations



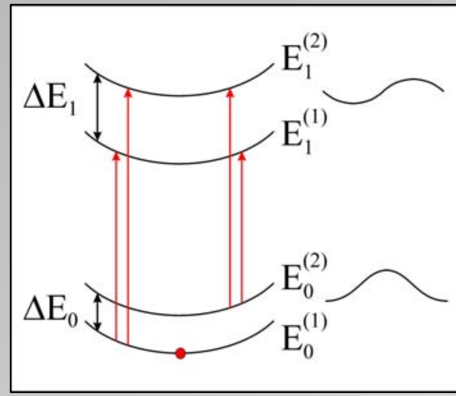




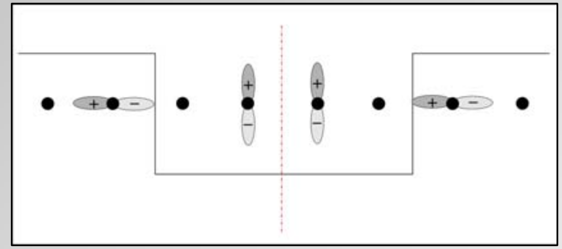
Silicon



Germanium

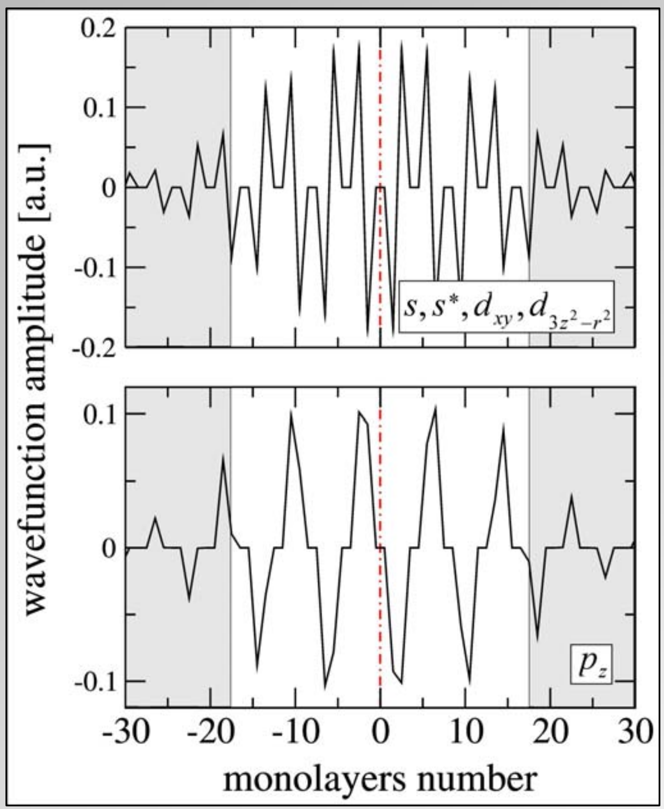


$E_1^{(2)}$
ΔE_1
$E_1^{(1)}$
$E_0^{(2)}$
ΔE_0
$E_0^{(1)}$

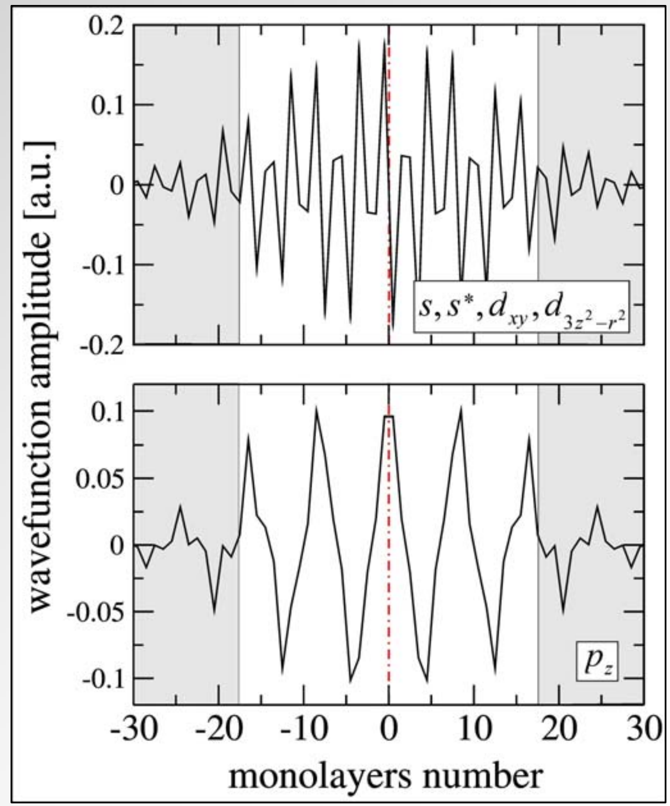


$E_0^{(1)}$

$E_0^{(2)}$

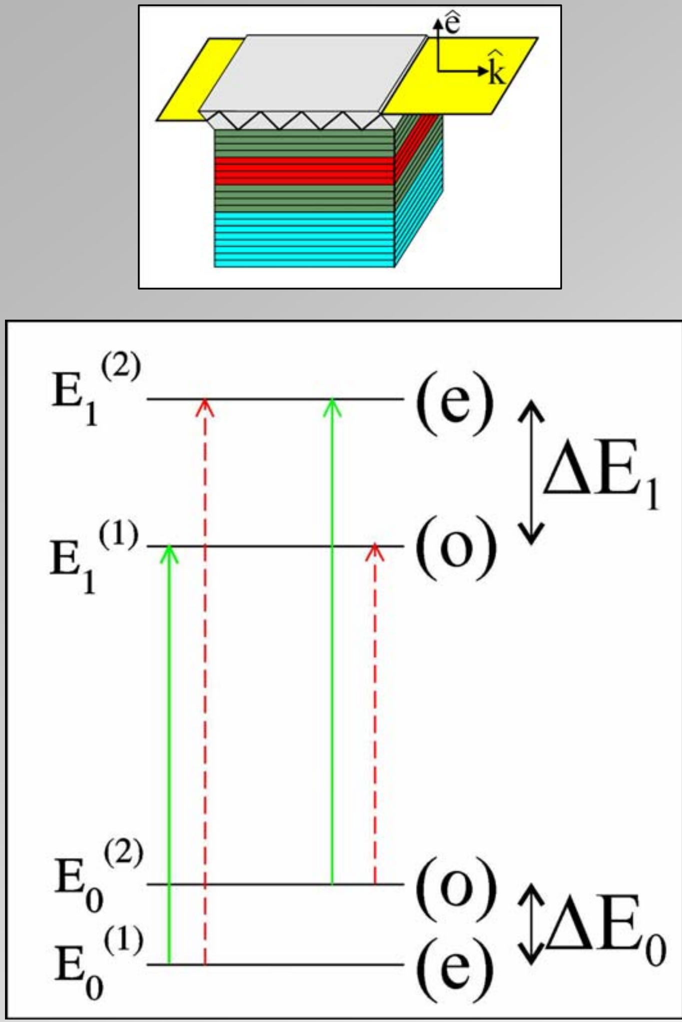


wavefunction amplitude [a.u.]
$s, s^*, d_{xy}, d_{3z^2-r^2}$
p_z
monolayers number

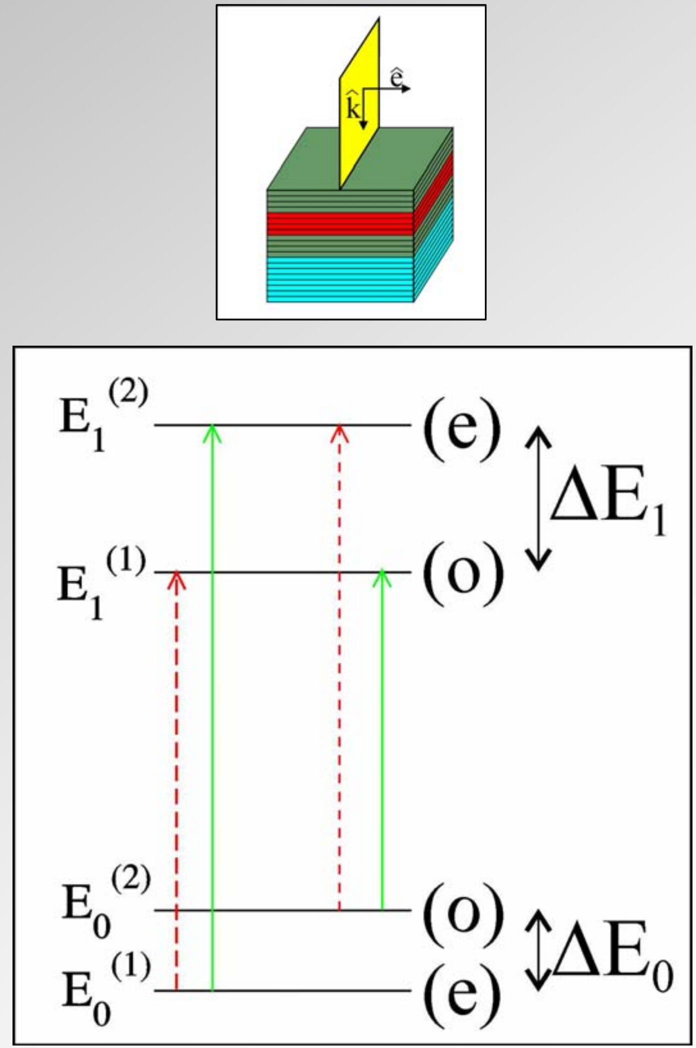


wavefunction amplitude [a.u.]
$s, s^*, d_{xy}, d_{3z^2-r^2}$
p_z
monolayers number

Selection rules

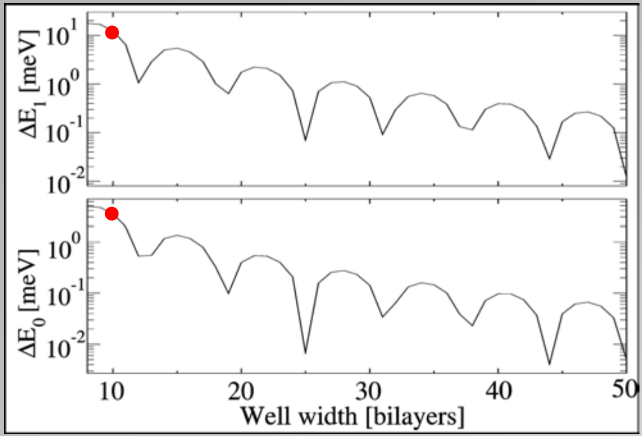


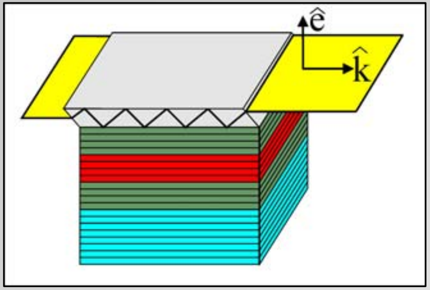
Silicon and Germanium

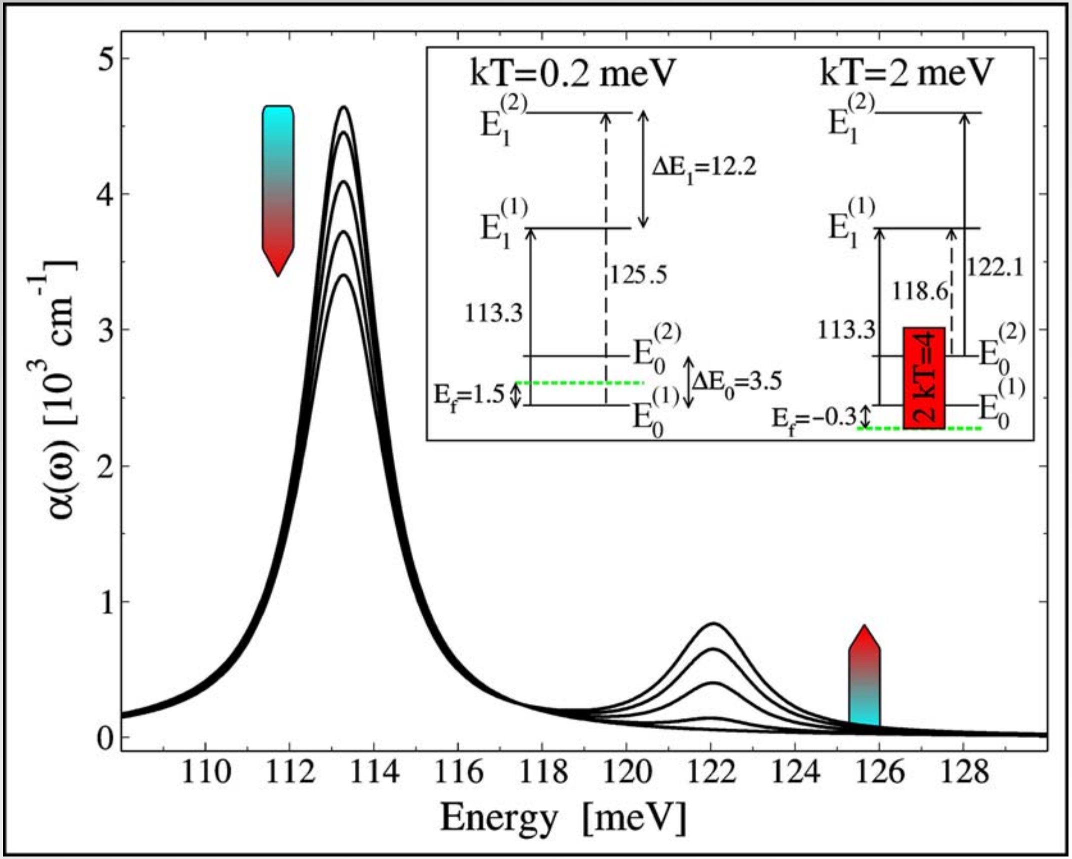


Germanium

Silicon intersubband absorption

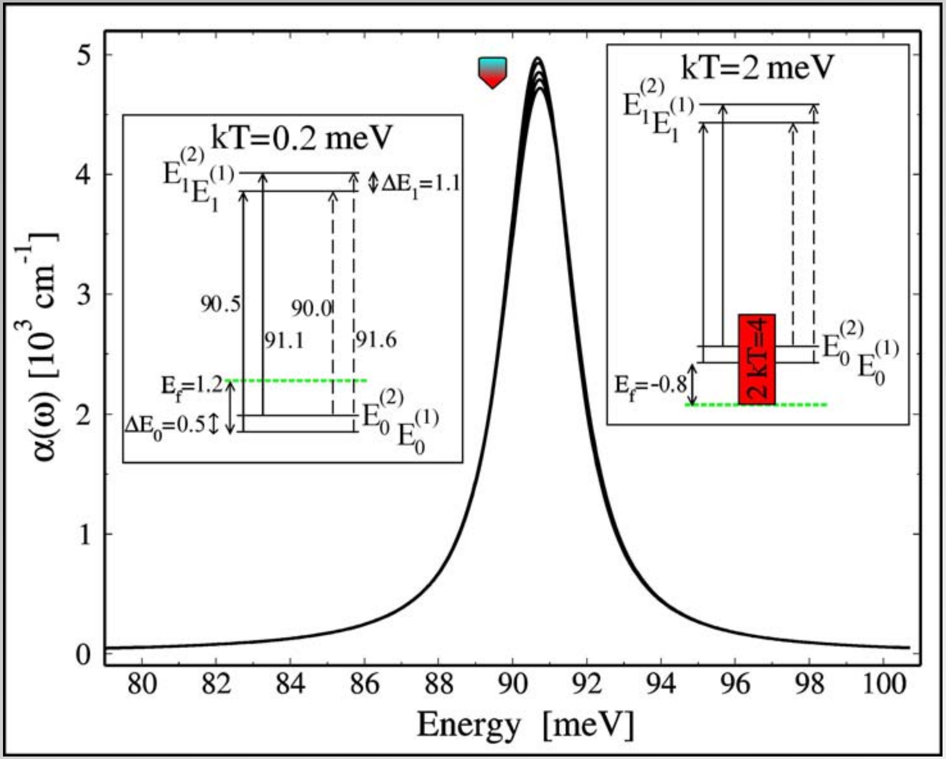


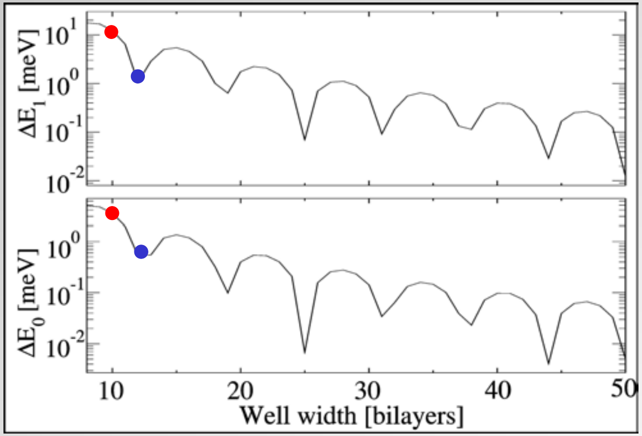


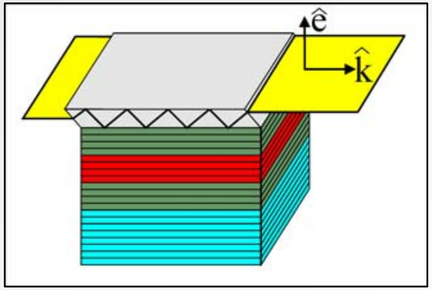


M. Virgilio and G. Grosso, Phys. Rev. B, **75**, 235428 (2007)

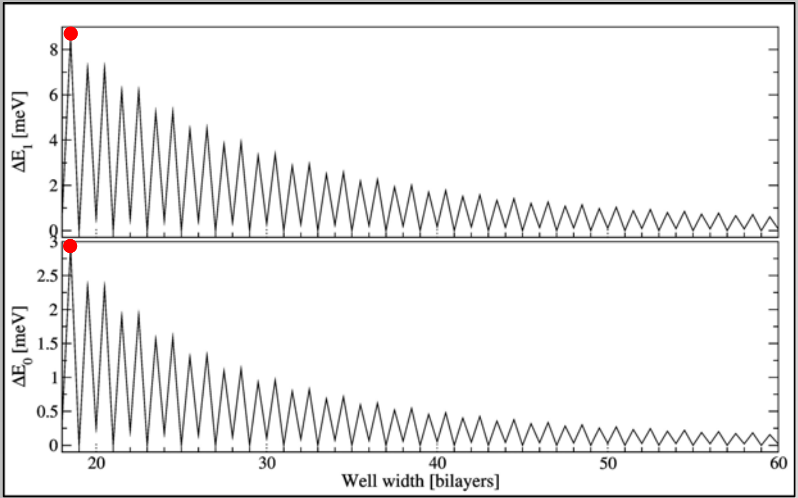
Silicon intersubband absorption

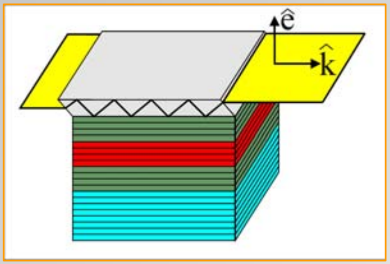


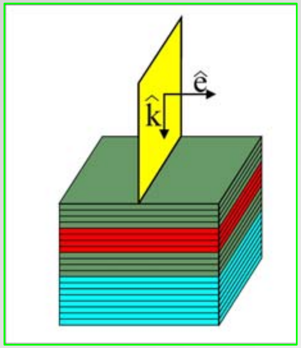


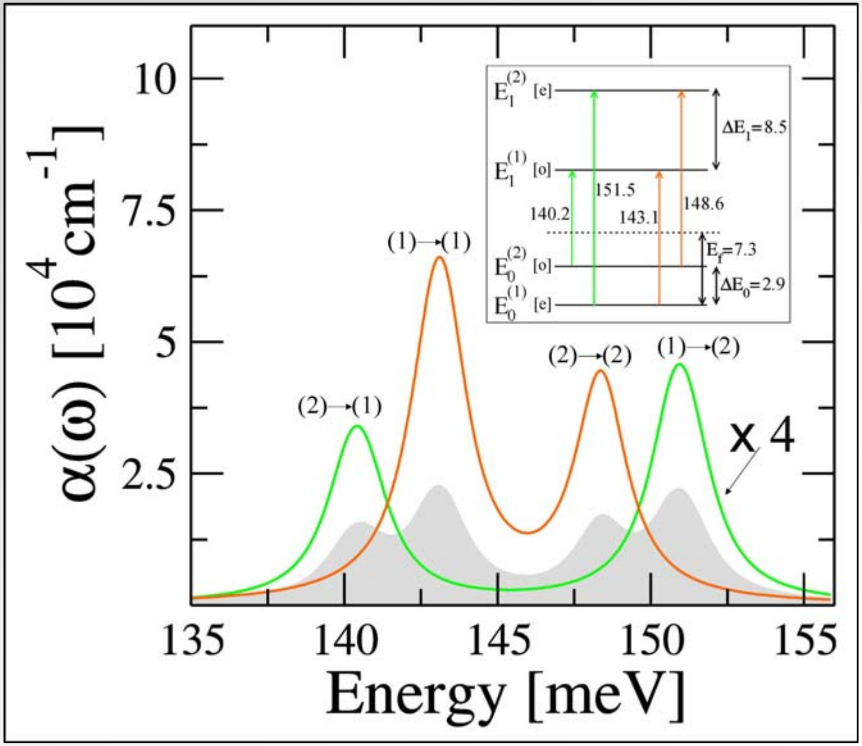


Germanium intersubband absorption

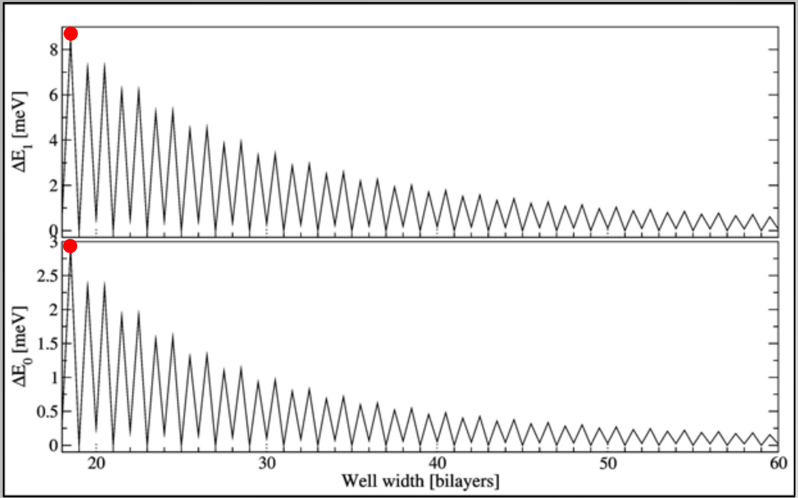


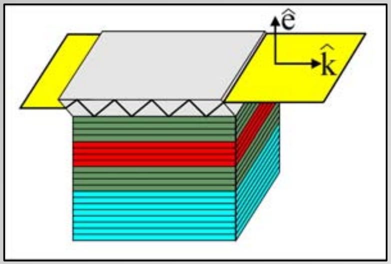


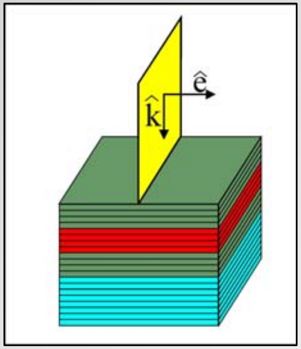


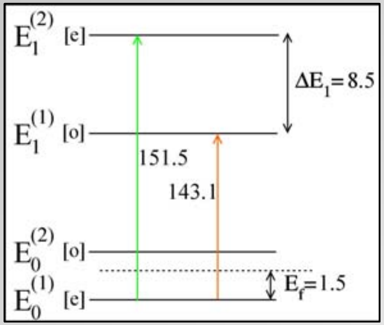


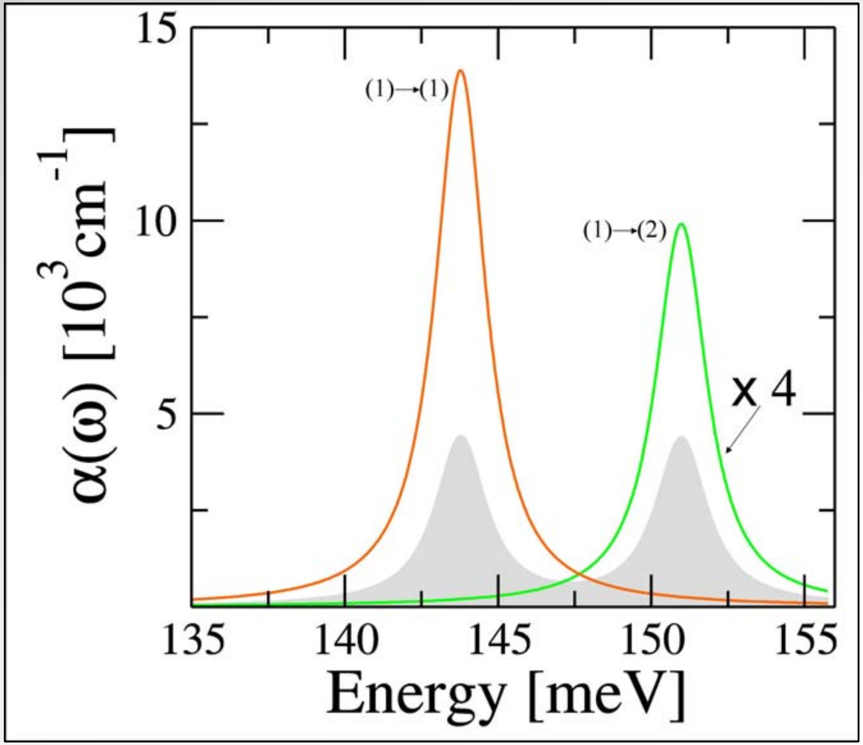
Germanium intersubband absorption





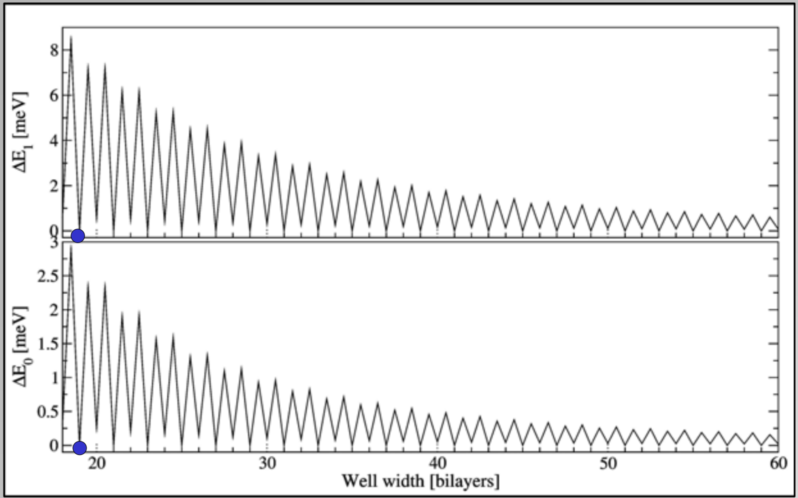


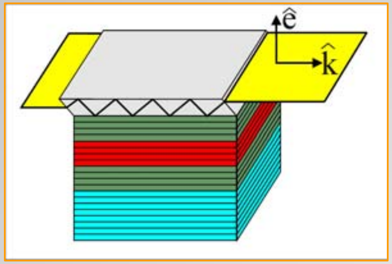


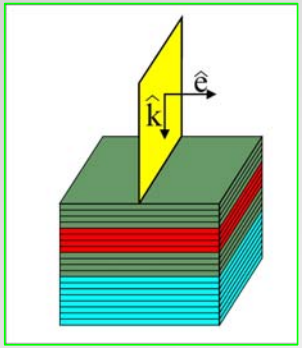


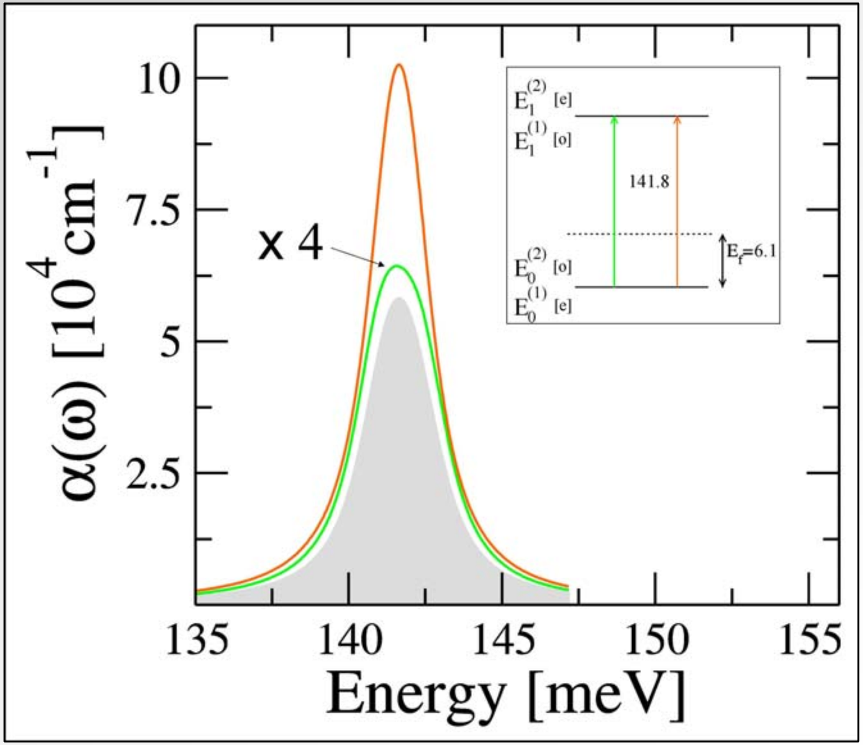
Optical measurement of valley splitting

Germanium intersubband absorption

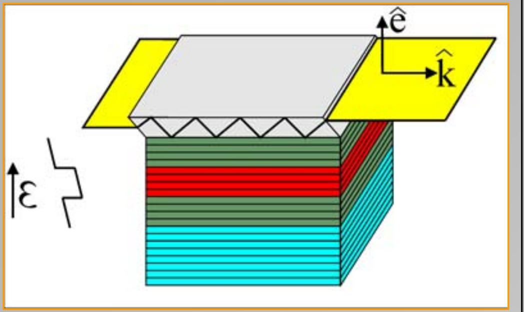


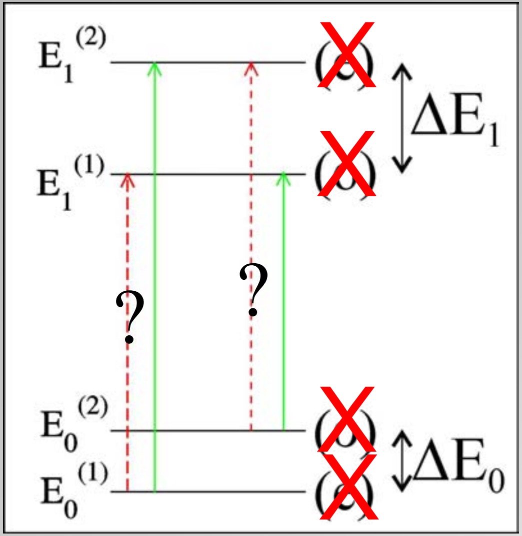




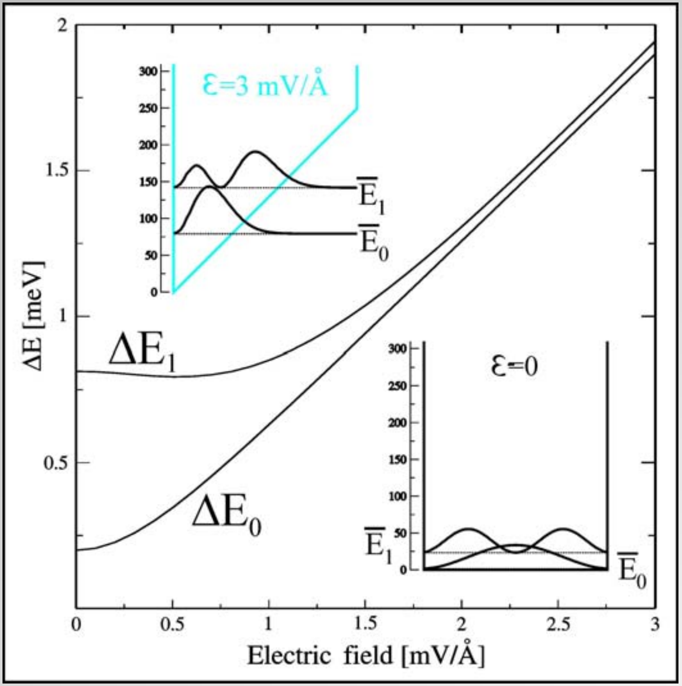


Silicon

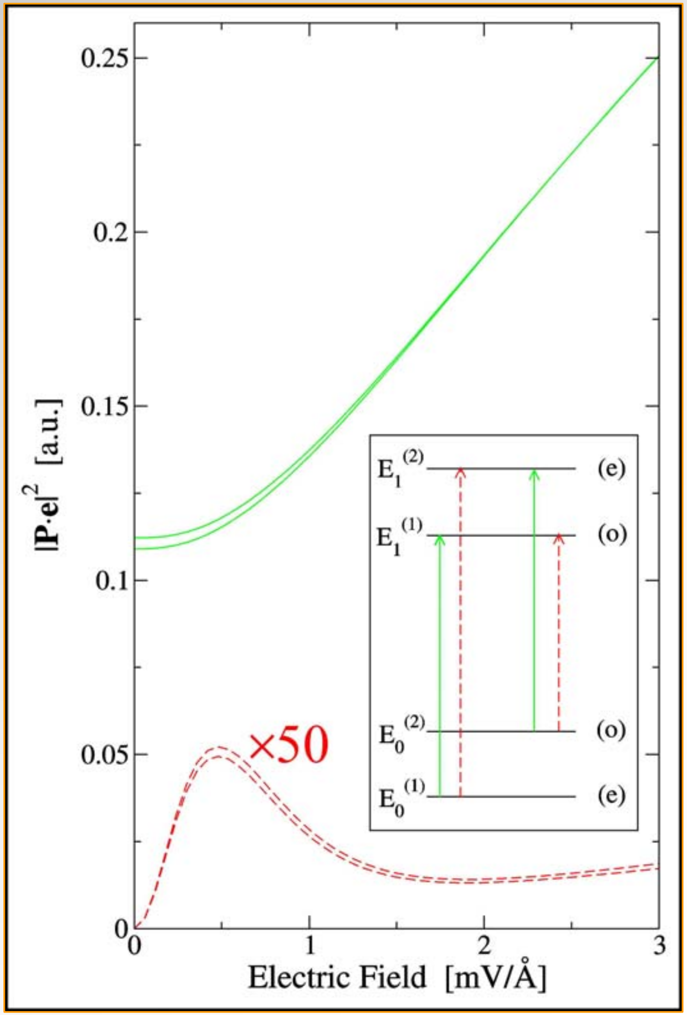




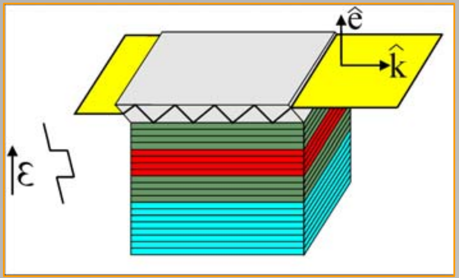
$E_1^{(2)}$
$E_1^{(1)}$
$E_0^{(2)}$
$E_0^{(1)}$
?
?
ΔE_1
ΔE_0



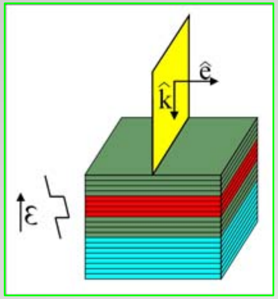
ΔE [meV]
Electric field [mV/Å]
ΔE_1
ΔE_0
Ɛ=3 mV/Å
Ɛ=0
$\overline{E}_1$
$\overline{E}_0$

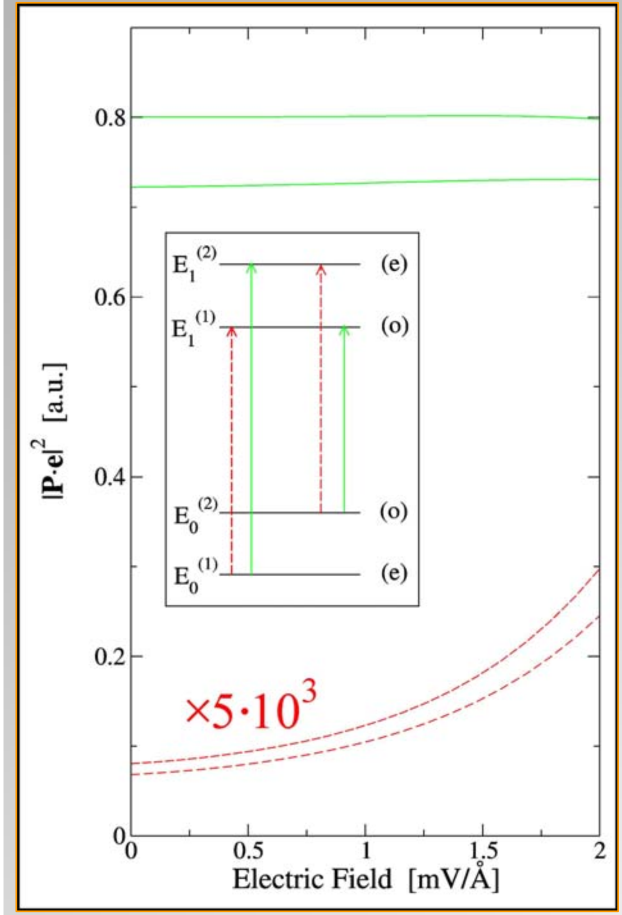


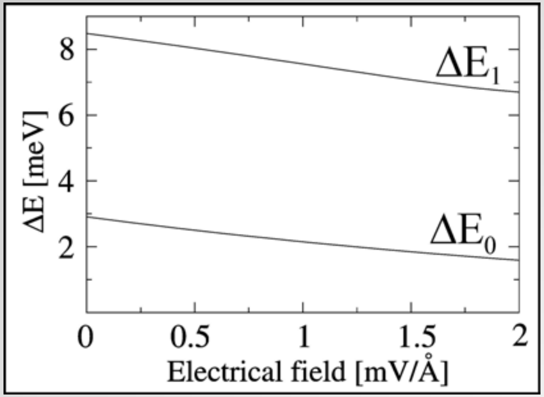
$|\mathbf{P}\cdot\mathbf{e}|^2$ [a.u.]
Electric Field [mV/Å]
×50
$E_1^{(2)}$ (e)
$E_1^{(1)}$ (o)
$E_0^{(2)}$ (o)
$E_0^{(1)}$ (e)

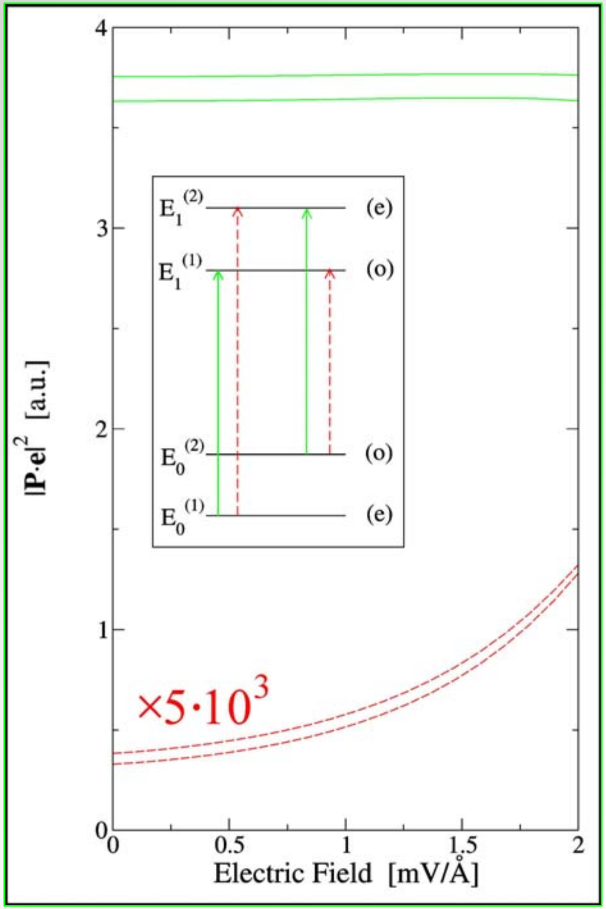

ê
k̂
ε

Germanium


ê
k̂
ε


|P·e|² [a.u.]
0.8
0.6
0.4
0.2
0
0.5
1
1.5
2
Electric Field [mV/Å]
E1(2) (e)
E1(1) (o)
E0(2) (o)
E0(1) (e)
×5·10³

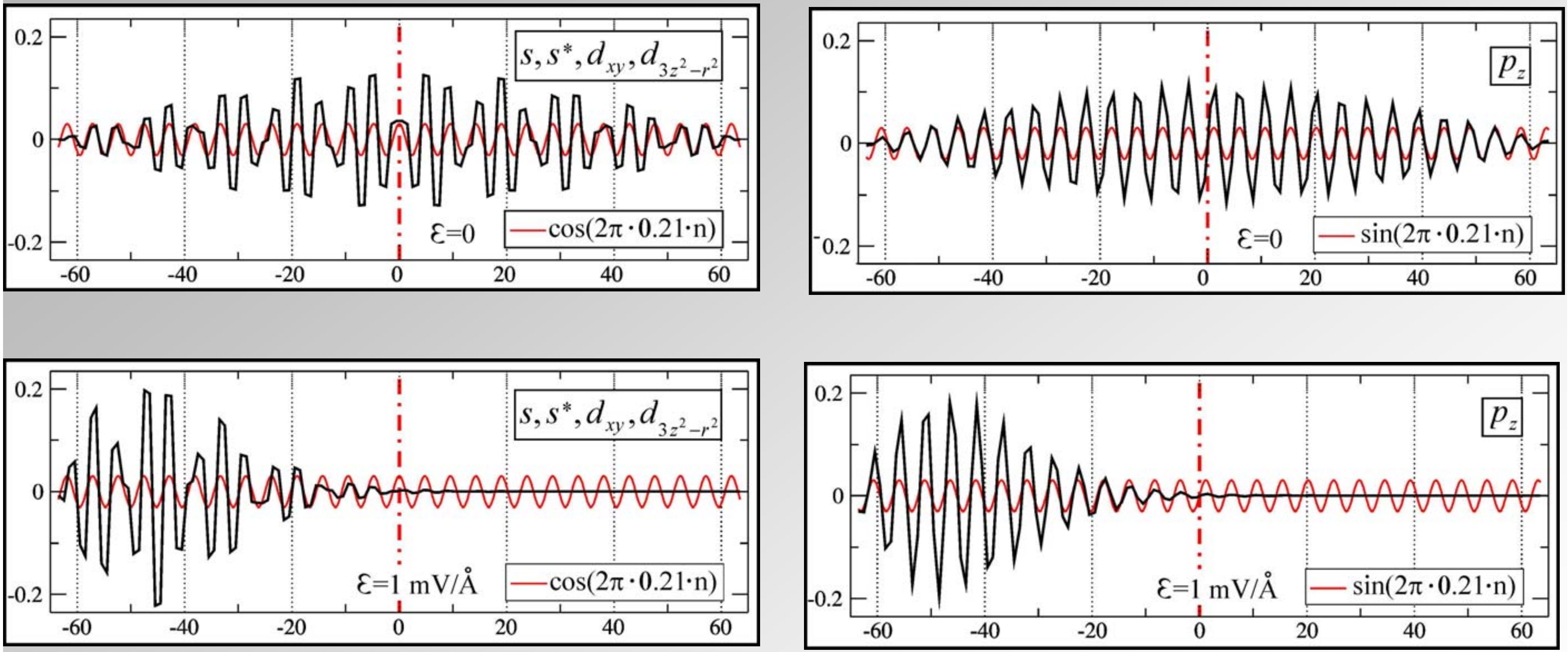

ΔE [meV]
8
6
4
2
ΔE1
ΔE0
0
0.5
1
1.5
2
Electrical field [mV/Å]


|P·e|² [a.u.]
4
3
2
1
0
0.5
1
1.5
2
Electric Field [mV/Å]
E1(2) (e)
E1(1) (o)
E0(2) (o)
E0(1) (e)
×5·10³

Conclusions

- Electronic states and optical properties (intraband+intersubband) of SiGe QWs with tight-binding Hamiltonian
- Valley splitting in SiGe QW structures
- Signatures of intervalley splitting in the intersubband absorption spectrum
- Optical measurement of valley splitting

Selection rules with electric field



$$E_0^{(1)}$$

Method (III): dipole operator in the tight-binding model

$$\langle \Psi^f(\vec{k},\vec{r})|\hat{\epsilon}\cdot\vec{p}|\Psi^i(\vec{k},\vec{r})\rangle = \hat{\epsilon}\cdot\vec{p}^{fi}(\vec{k})$$

$$\vec{p}^{fi}(\vec{k}) = \sum_{m,l}\sum_{\mu,\nu} A_m^{\mu *}(\vec{k},f) A_l^{\nu}(\vec{k},i) \sum_n e^{ik_z\tau_{nz}} e^{\vec{k}_{\parallel}\cdot(\vec{\tau}_n+\vec{d}_\nu-\vec{d}_\mu)} \langle \phi_m(\vec{r}-\vec{d}_\mu)|\vec{p}|\phi_l(\vec{r}-\vec{\tau}_n-\vec{d}_\nu)\rangle$$

$$\vec{p} = \frac{m}{i\hbar}[\vec{r},H]$$

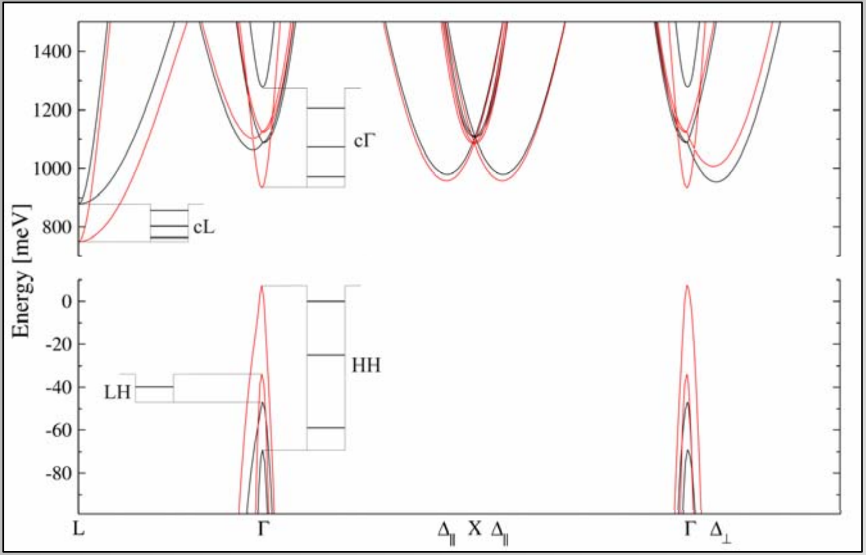
$$\langle \phi_m(\vec{r}-\vec{d}_\mu)|\vec{r}|\phi_l(\vec{r}-\vec{\tau}_n-\vec{d}_\nu)\rangle \simeq \delta_{m,l}\delta_{\vec{d}_\mu,\vec{\tau}_n+\vec{d}_\nu}(\vec{\tau}_n+\vec{d}_\nu)$$

$$\begin{aligned}\hat{\epsilon}\cdot\vec{p}^{fi}(\vec{k}) \quad = \quad & \frac{m}{i\hbar}\sum_{m,l}\sum_{\mu,\nu} A_m^{\mu *}(\vec{k},f) A_l^{\nu}(\vec{k},i) \sum_n e^{ik_z\tau_{nz}} e^{\vec{k}_{\parallel}\cdot(\vec{\tau}_n+\vec{d}_\nu-\vec{d}_\mu)} \\ & \hat{\epsilon}\cdot(\vec{\tau}_n+\vec{d}_\nu-\vec{d}_\mu)\langle \phi_m(\vec{r}-\vec{d}_\mu)|H|\phi_l(\vec{r}-\vec{\tau}_n-\vec{d}_\nu)\rangle\end{aligned}$$

$$\hat{\epsilon}\cdot\vec{P} = \begin{pmatrix} \boxed{0} & \boxed{F_1} & 0 & \dots & \dots & \dots & 0 & e^{-ik_z l_z}F_2 \\ F_1^\dagger & 0 & \boxed{F_2} & 0 & \dots & \dots & \dots & 0 \\ 0 & F_2^\dagger & 0 & F_1 & 0 & \dots & \dots & 0 \\ 0 & 0 & F_1^\dagger & 0 & F_2 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & \dots & \dots & \dots & 0 & F_2^\dagger & 0 & F_1 \\ e^{ik_z l_z}F_2^\dagger & 0 & \dots & \dots & \dots & 0 & F_1^\dagger & 0 \end{pmatrix}$$

$$\alpha(\hbar\omega) = \frac{4\pi e^2\hbar}{n_0 c m_0^2 V\Gamma}\sum_{\vec{k}}\sum_{f,i}\frac{\hat{\epsilon}\cdot\vec{p}^{f,i}(\vec{k})}{E_f(\vec{k})-E_i(\vec{k})}\cdot\{f[E_i(\vec{k})]-f[E_f(\vec{k})]\}\cdot\frac{1}{1+(\frac{E_f-E_i-\hbar\omega}{\Gamma})^2}$$

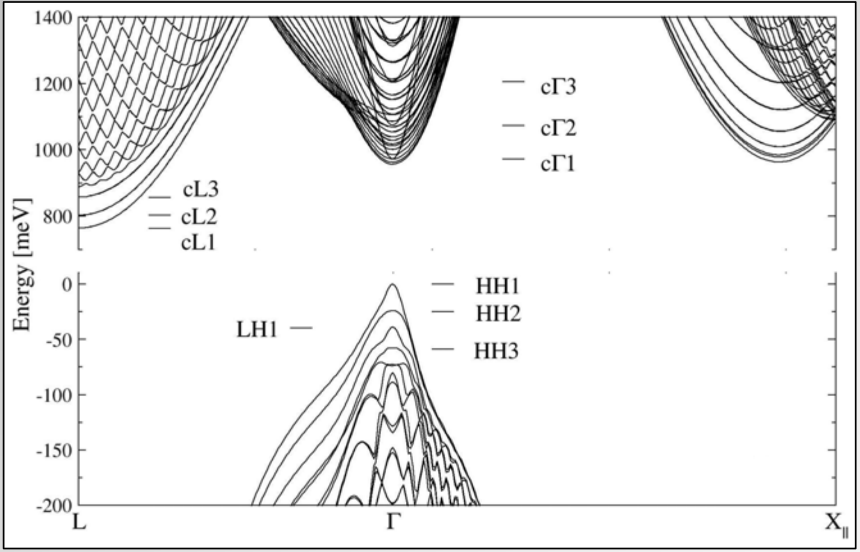
TB for interband transitions in SiGe QW

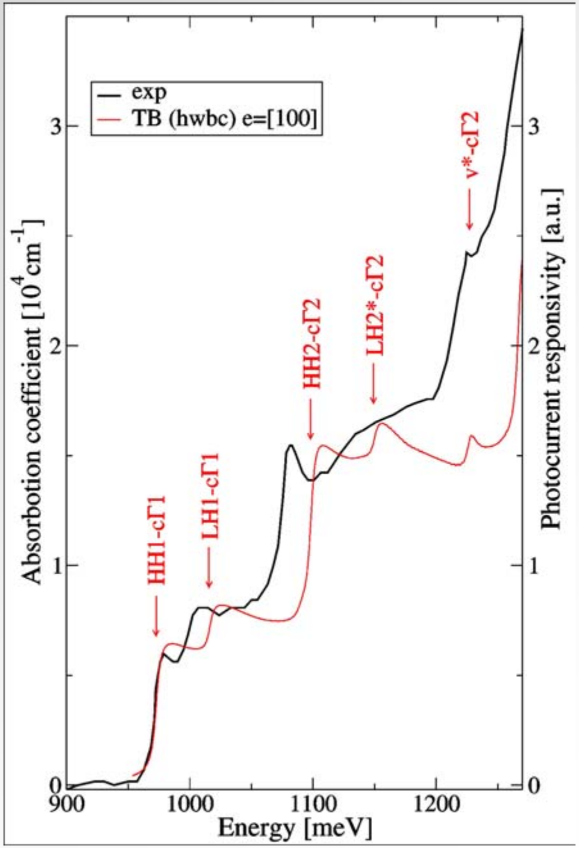


—— $Si_{0.15}Ge_{0.85}$

—— Ge

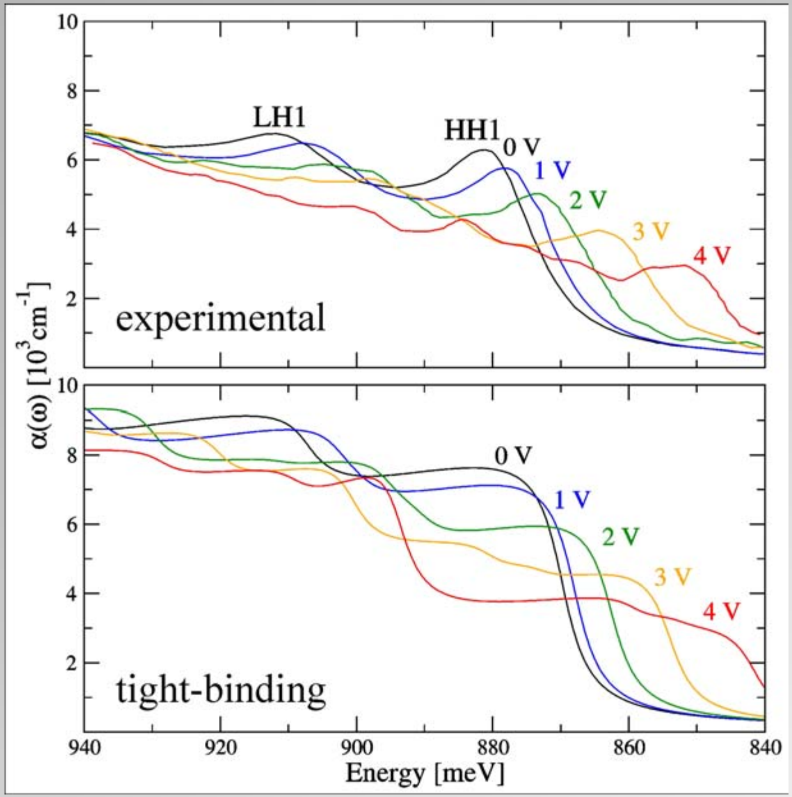
$Si_{0.1}Ge_{0.9}$ substrate

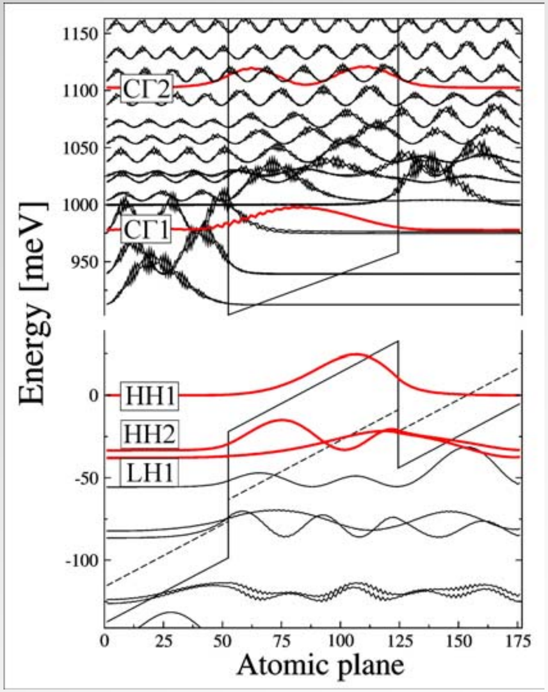




interband transitions in SiGe QW

QCSE



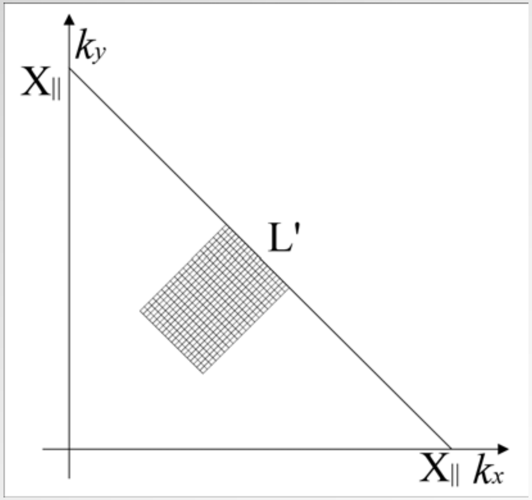


Dipole operator in the tight-binding model

$$\alpha(\hbar\omega) = \frac{4\pi e^2\hbar}{n_0 c m_0^2 V\Gamma} \sum_{\vec{k}} \sum_{f,i} \frac{\hat{\epsilon}\cdot\vec{p}^{f,i}(\vec{k})}{E_f(\vec{k}) - E_i(\vec{k})} \cdot \{f[E_i(\vec{k})] - f[E_f(\vec{k})]\} \cdot \frac{1}{1+(\frac{E_f - E_i - \hbar\omega}{\Gamma})^2}$$

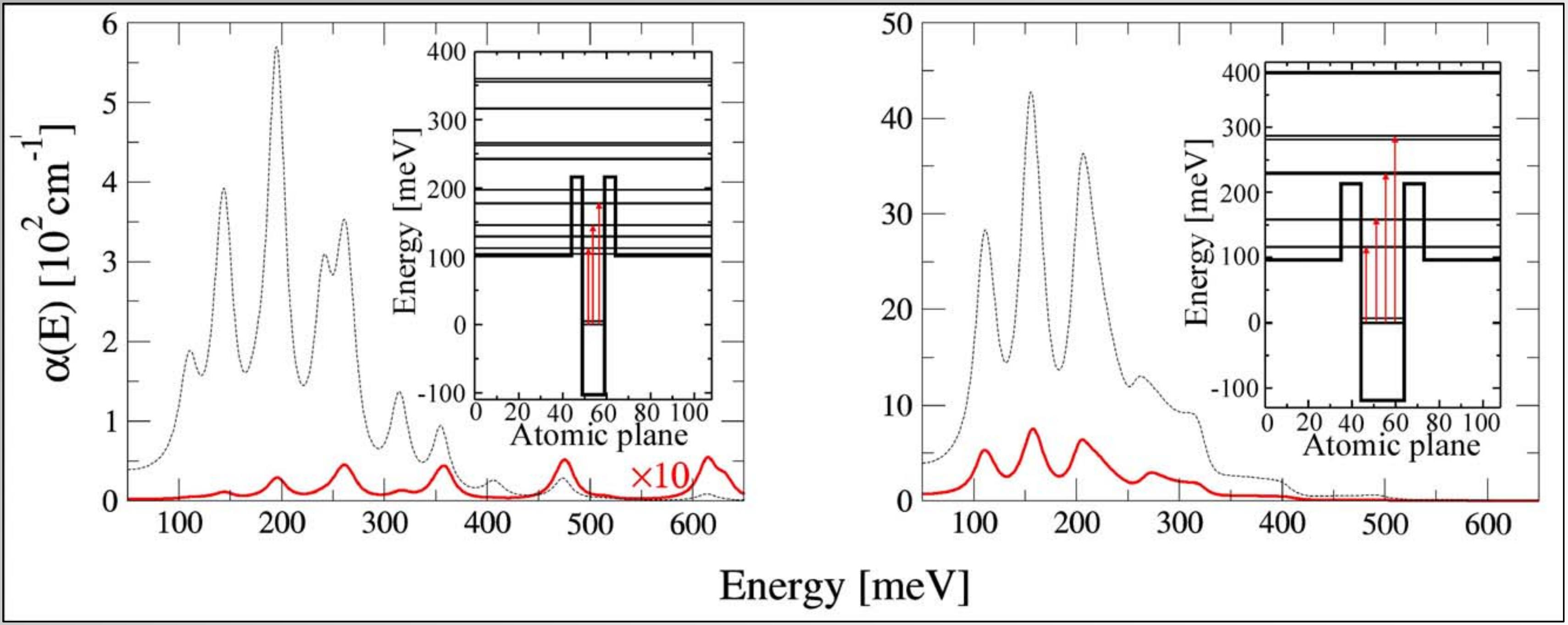
$$\langle\Psi^f(\vec{k},\vec{r})|\hat{\epsilon}\cdot\vec{p}|\Psi^i(\vec{k},\vec{r})\rangle = \hat{\epsilon}\cdot\vec{p}^{fi}(\vec{k})$$

$$\vec{p}^{fi}(\vec{k}) = \sum_{m,l}\sum_{\mu,\nu} A_m^{\mu *}(\vec{k},f) A_l^{\nu}(\vec{k},i) \sum_n e^{ik_z\tau_{nz}} e^{\vec{k}_{\parallel}\cdot(\vec{\tau}_n+\vec{d}_\nu-\vec{d}_\mu)} \langle\phi_m(\vec{r}-\vec{d}_\mu)|\vec{p}|\phi_l(\vec{r}-\vec{\tau}_n-\vec{d}_\nu)\rangle$$



Conduction intersubband absorption at normal incidence

Bound to continuum transitions



Silicon

$$m_{xz}, m_{yz} = 0$$

Germanium

$$m_{xz}, m_{yz} \neq 0$$