Oxygen Defects in Silicon

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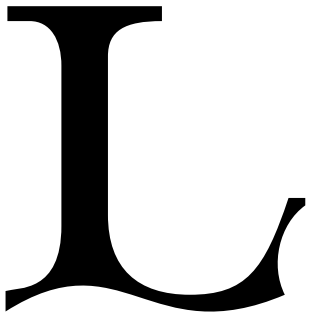


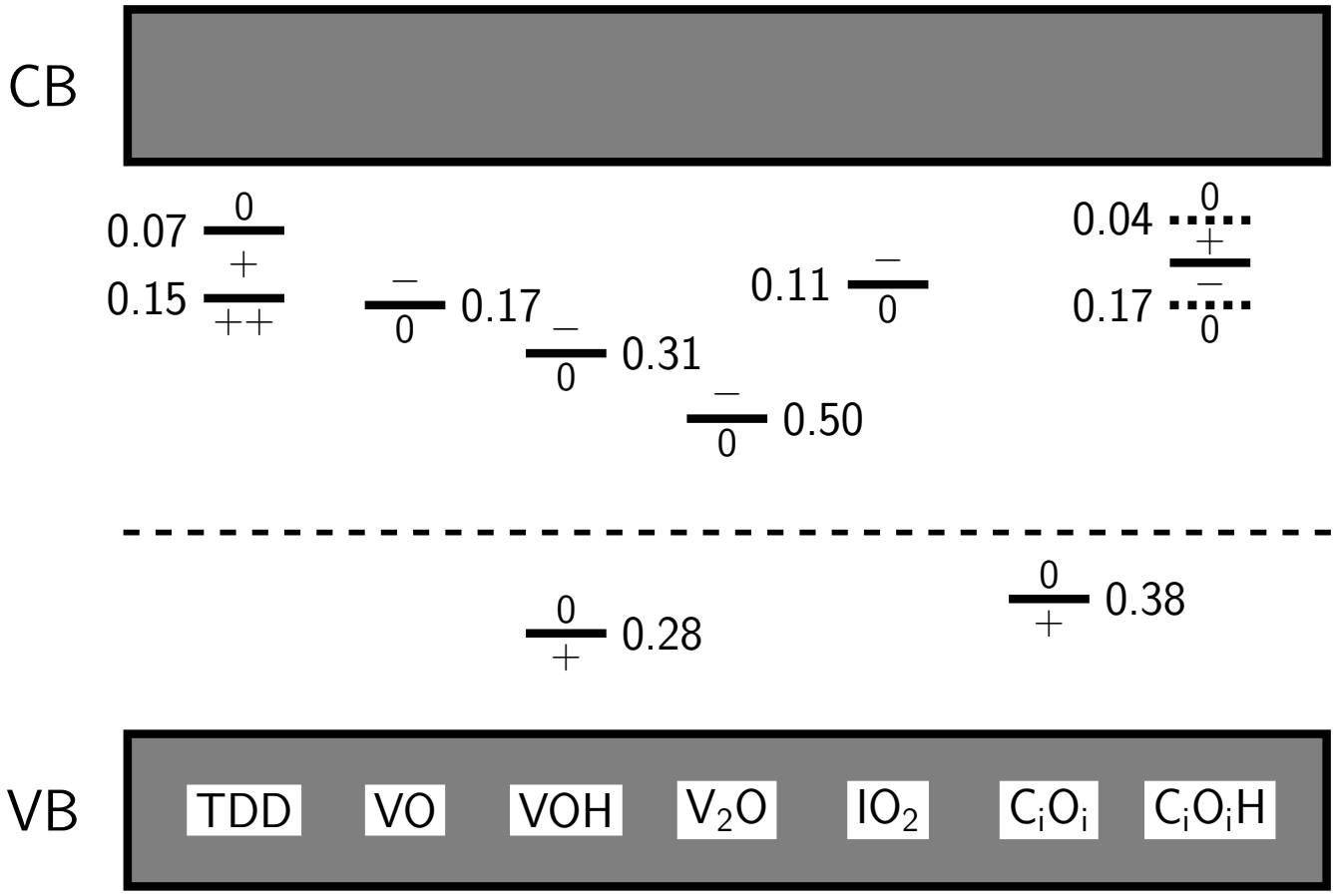
Contents

1. **Oxygen dimers and thermal donors**[1]**;**
2. **Oxygen-radiation and impurity defects;**

Density functional supercell code (AIMPRO**): evaluates structure, energetics, diffusion energies, LVMs, energy levels, piezo-spectroscopic B-tensor ($\Delta E = \mathrm{Tr}\, B \cdot \epsilon$)**

[1] Coutinho *et al.* Phys. Rev. Lett. **87**, 235501 (2001).

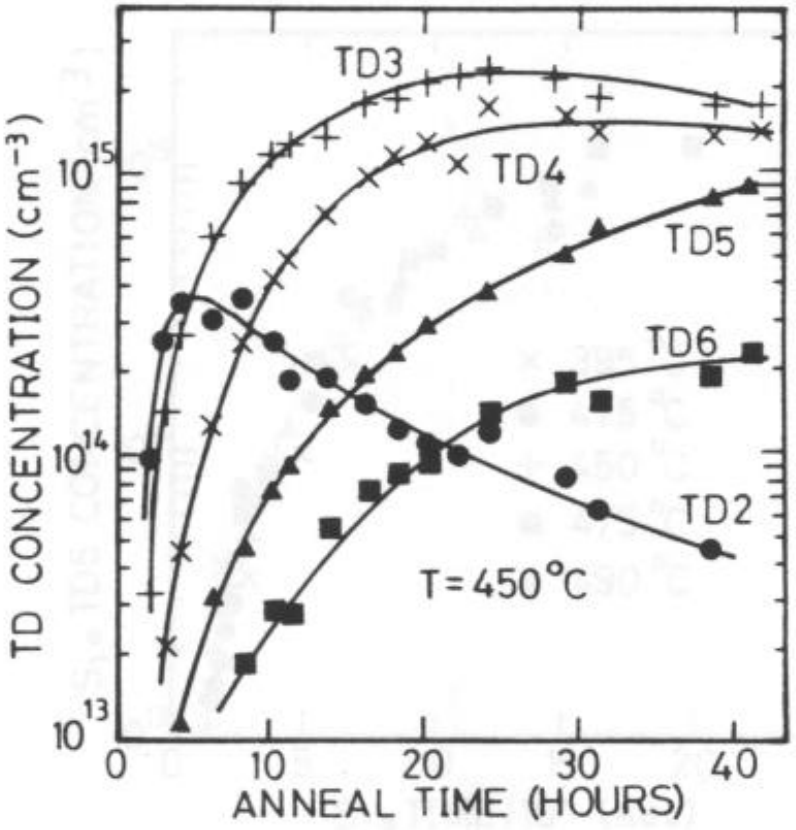
Energy levels of oxygen defects



Thermal donors - background

Heat treatments ($< 550°$C) of CZ-Si produce family of $\sim$ 16 double donors TDD(N)

- **formed sequentially**
- **increasingly shallow levels**
- **labelled NL8**

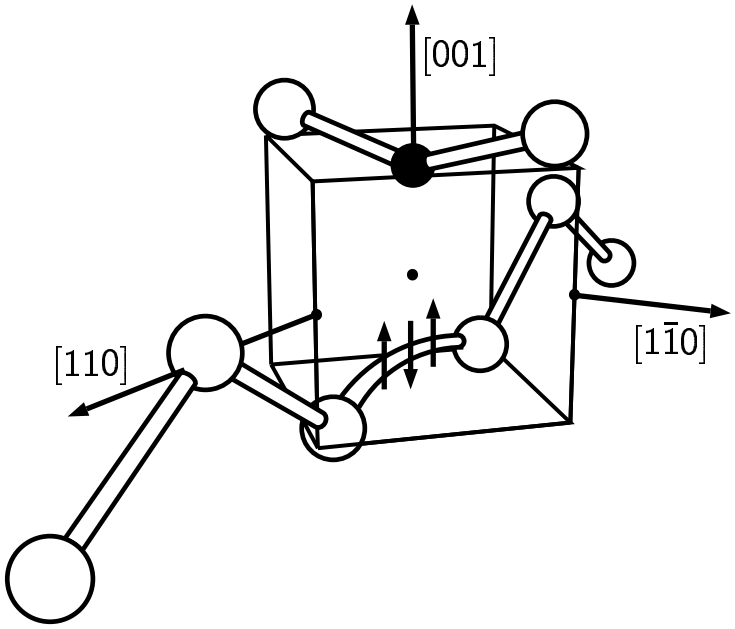


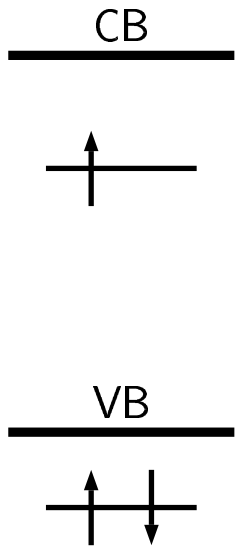
Troublesome Data

1. **Growth kinetics**
   - **TDD(1) $\rightarrow$ TDD(2), $Q \sim$ 1.2 eV**
   - **TDD(3) $\rightarrow$ TDD(4), $Q \sim$ 1.8 eV**
   - **Contrast oxygen diffusion energy ~ 2.5 eV**
2. **At most two oxygen related vibrational modes assigned to each donor.**

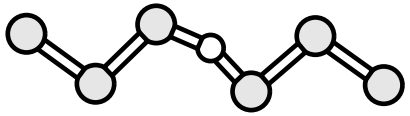
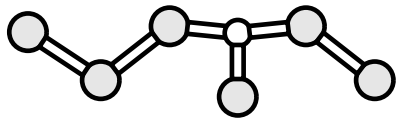
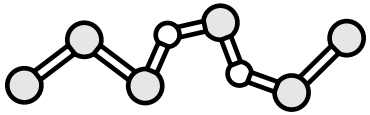
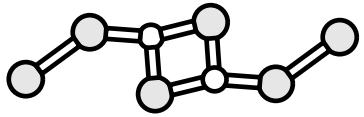
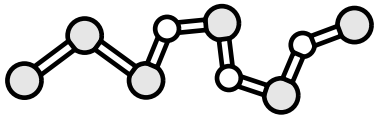
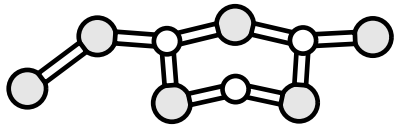
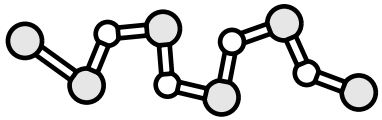
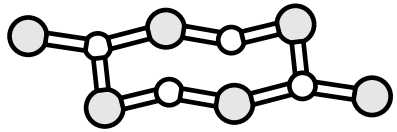
EPR/ENDOR: NL8

- TDD(N)$^+$: C_{2v} symmetry
- O^{17} -hyperfine data show two shells of oxygen atoms for first two donors.
- None with pure axial component.
- Largest $a \sim 0.52$ MHz, contrast VO^- where $a \sim$ 3 MHz.



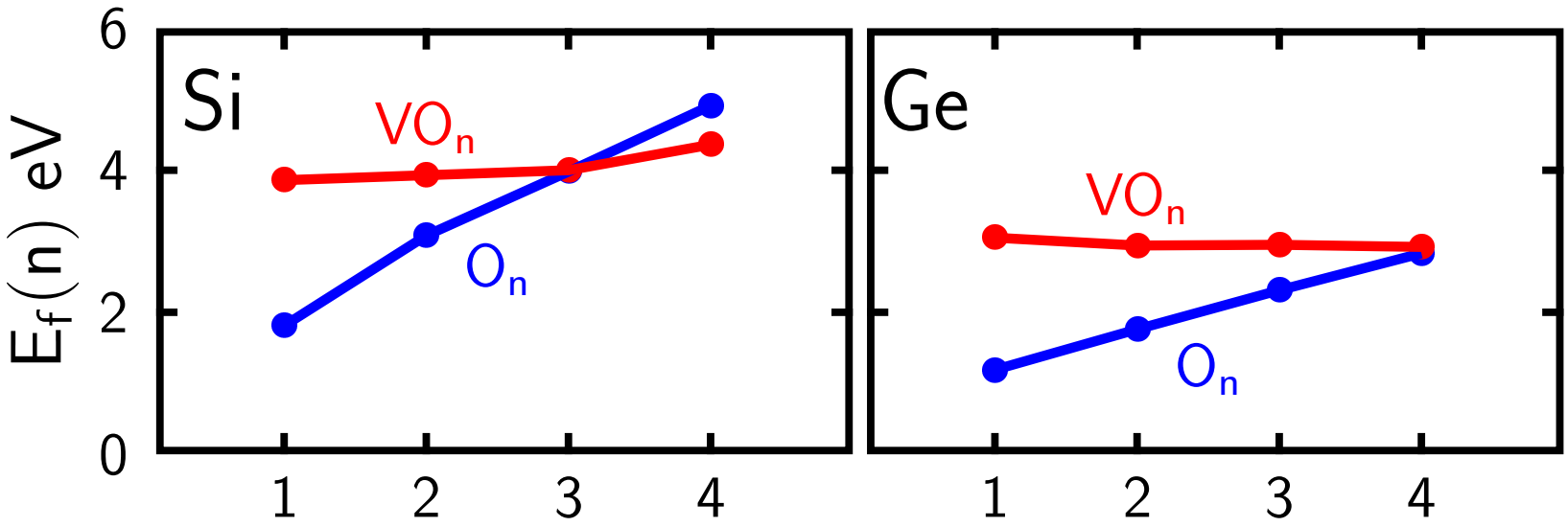


Diffusion energy

Si	Ge	Ground State	Saddle Point
2.2	1.7		
1.4	1.1		
1.3	1.1		
1.2	1.0		

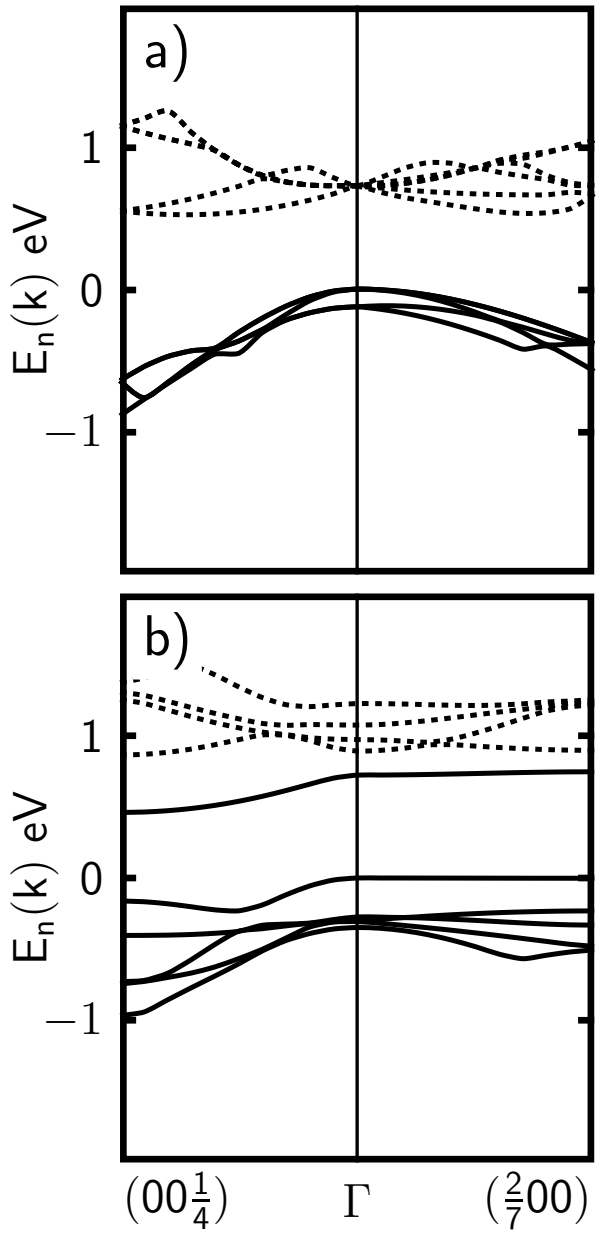
Diffusion energy (eV) of [110] O_n chains in 96 Si atom cells

Interstitial Generation

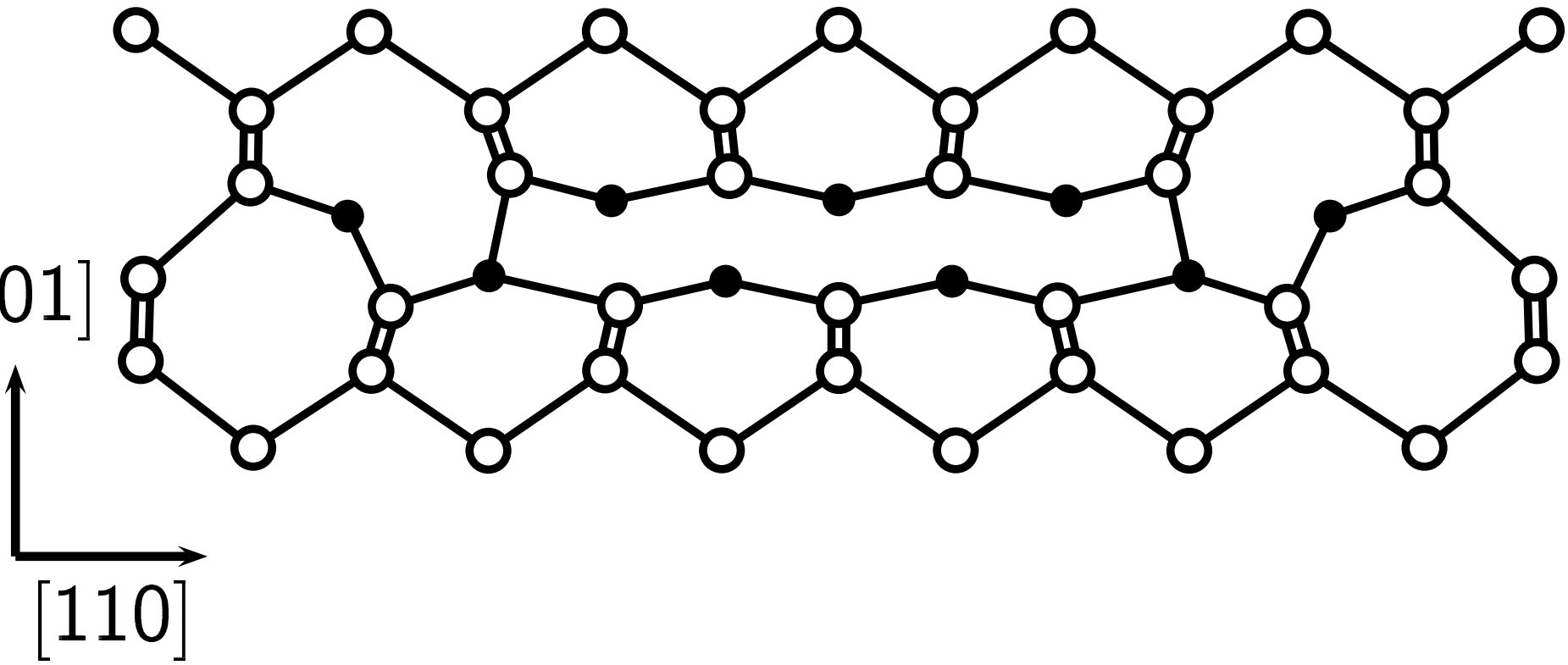


- **Interstitial production exothermic for $n > 4$**
- **Activation barrier $>$ 3.4 eV in Si.**

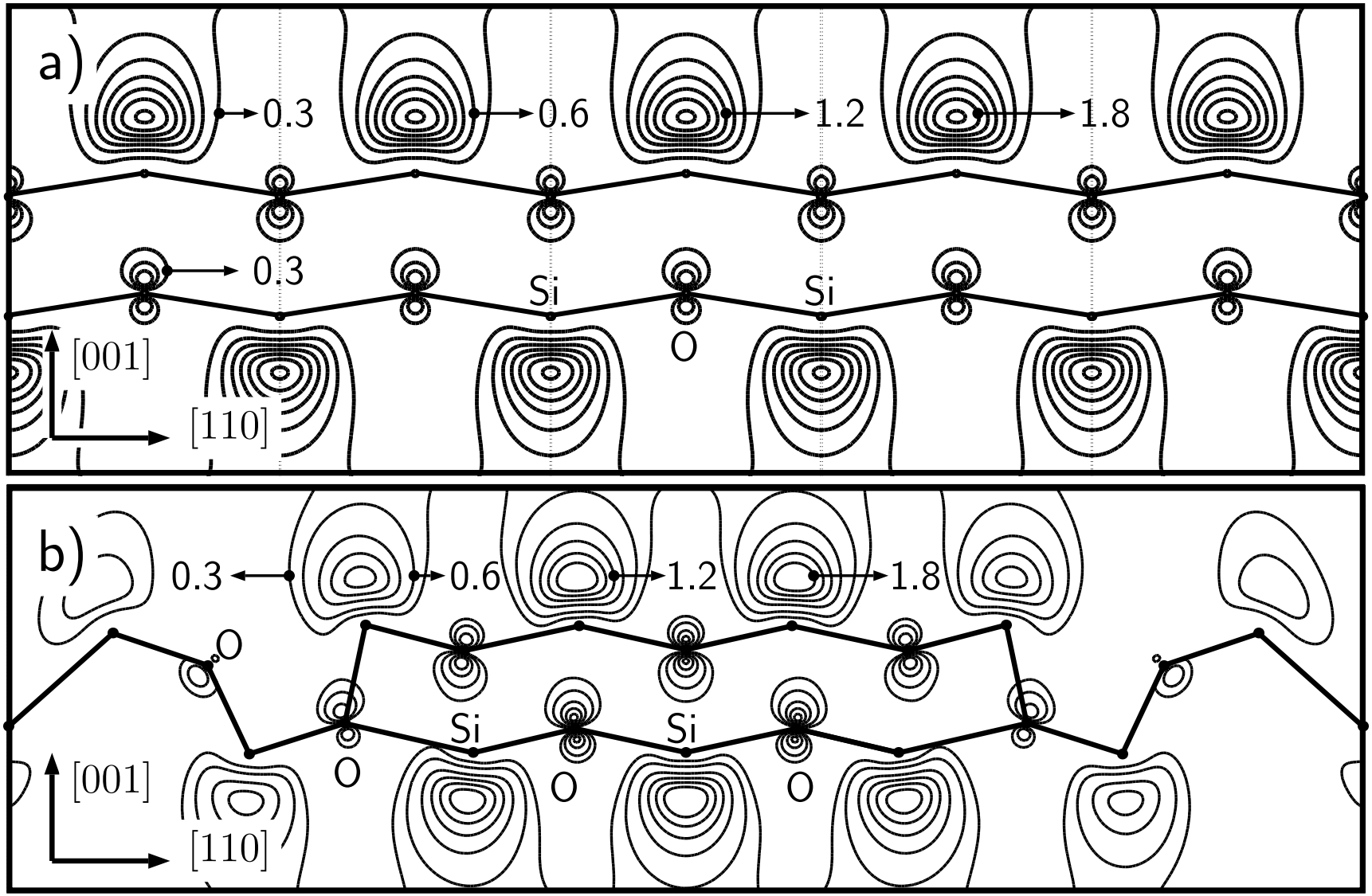
Band structure of a) Si and b) O_9 in 112 Si supercells



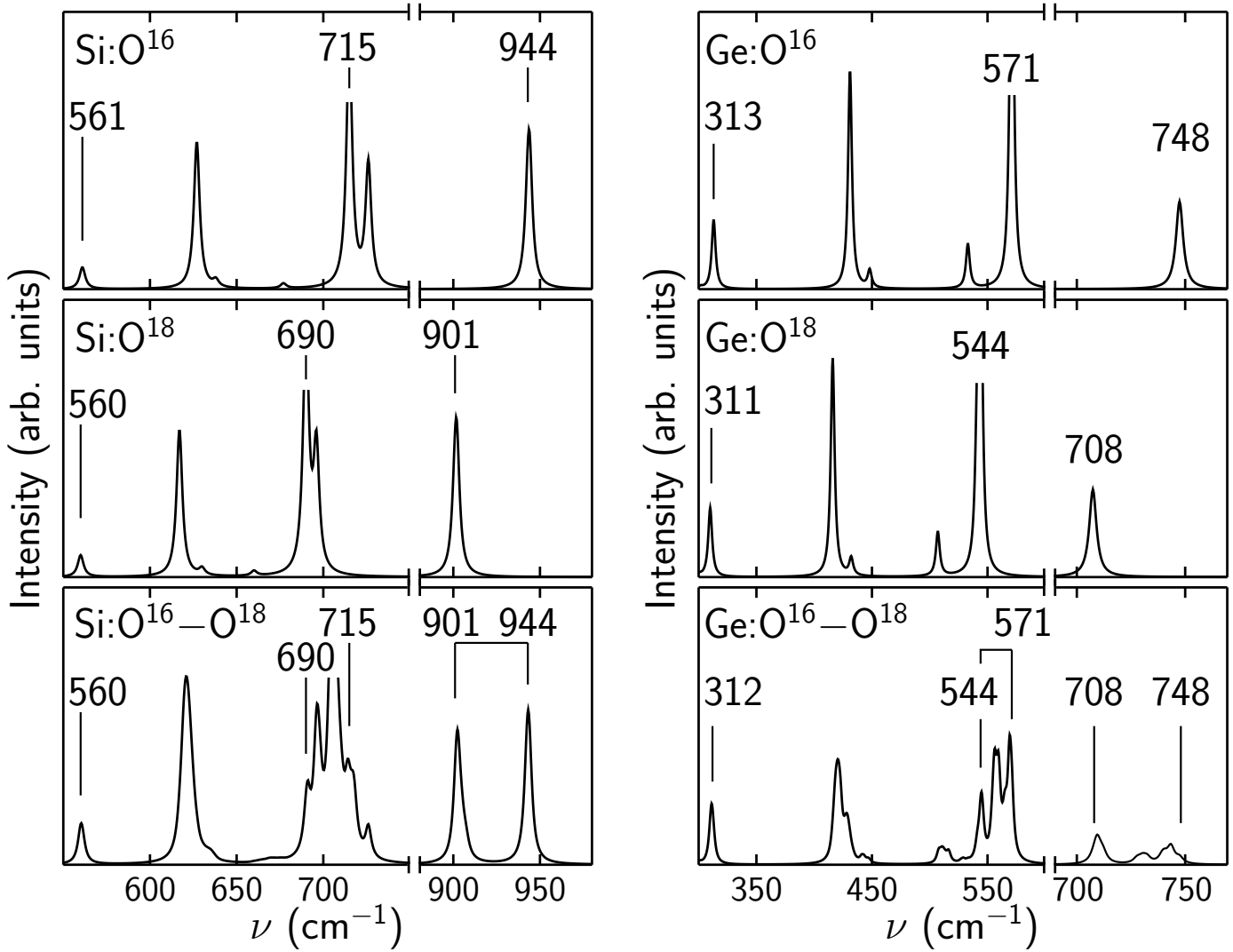
TDD model: O_9-2NN $\leftrightarrow$ TDD(4)



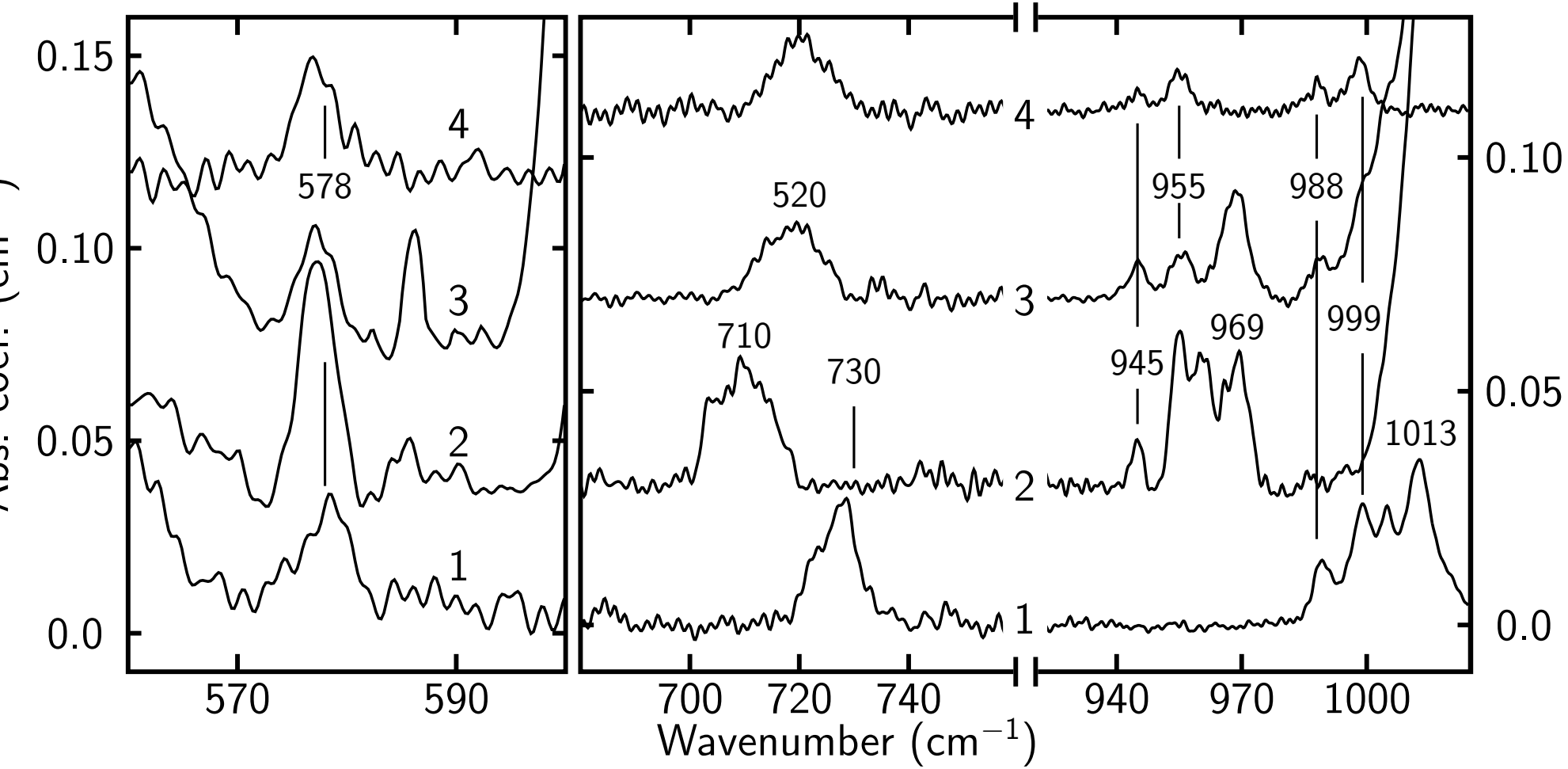
|Wavefunction|$^2 \times 1000$ of (a) LUB in O_∞, (b) HOB in O_9



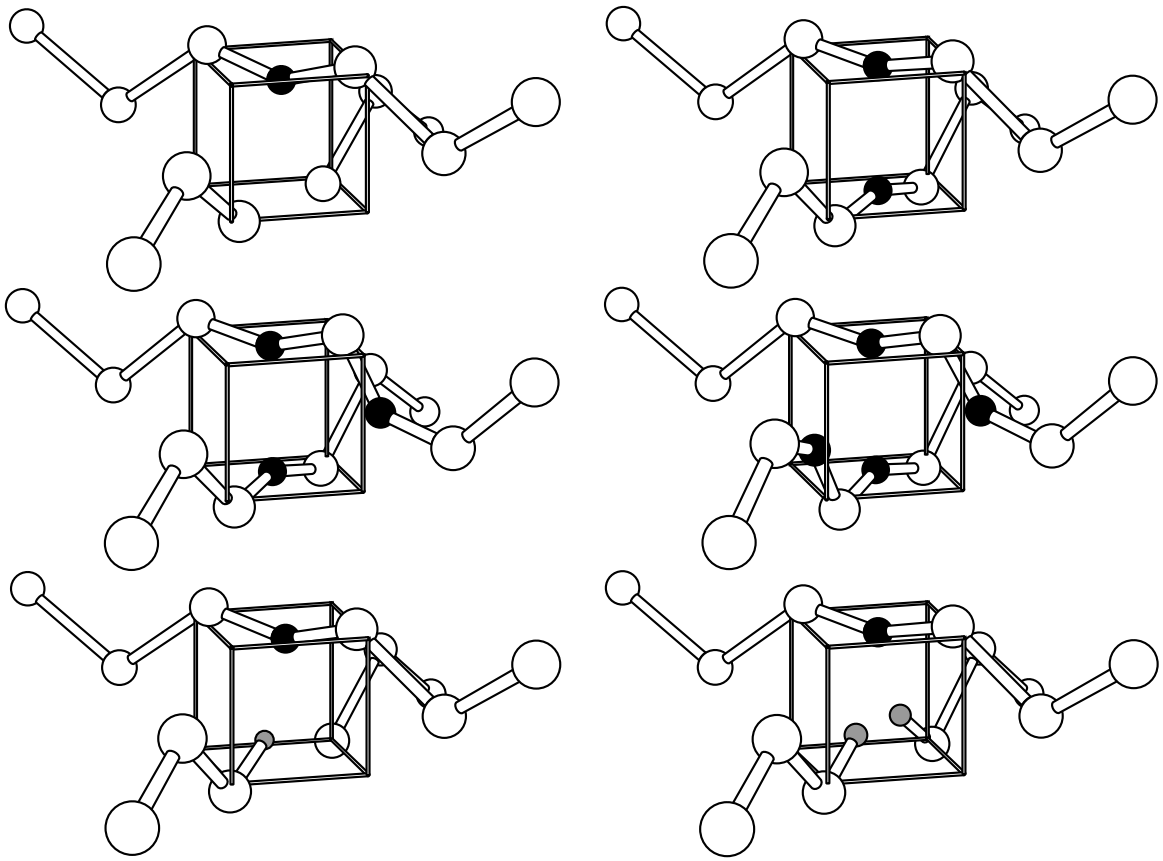
Thermal Donors LVMs, $O_7 \leftrightarrow$TDD(2)



Measurements in Si

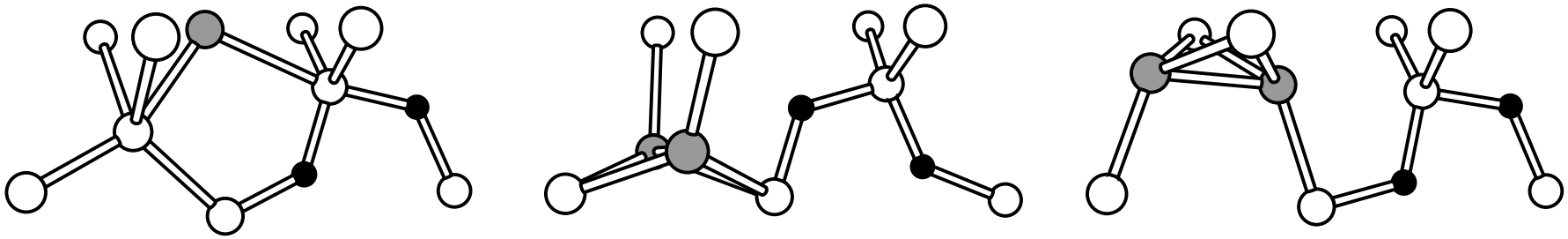


VO_n and VOH_n defects



VO_2, VO_3, VO_4 and VOH_2 passive

Self-interstitial oxygen defects

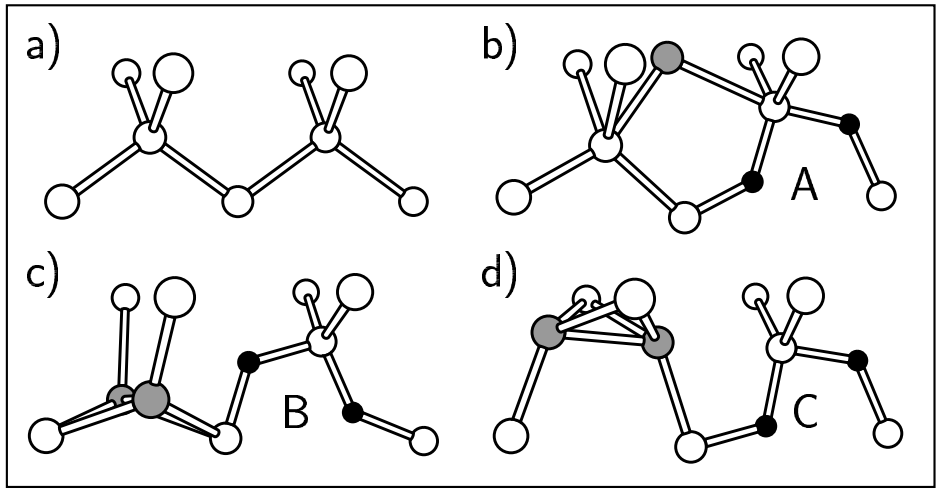


IO_2^+ IO_2^0 IO_2^-

- I**O stable up to** $T \leq$**300 K;**
- $I\mathrm{O}_2$ **stable up to 180°C.**

$I\mathrm{O}_2$ defect

Ground state structures



Defect	E_b (eV)
A	0.39
B	0.75
C	0.63

Binding energy of I^0 with O_2 is 0.75 eV.

Lindström em et al. Physica B, *in press.*

- **Samples: n-type, C-lean Cz-Si, with ^{16}O or ^{18}O species;**
- **Hot e-irradiation (2.5 MeV) up to 650 K: enhancement of $I + V\mathrm{O}_2 \rightarrow \mathrm{O}_{2i}$;**
- $[\mathrm{O}_{2i}] \sim 5 \times 10^{16}$**cm**$^{-3}$**;**

- **Further e-irradiation at 300K leading to:**

$$I_{\mathrm{Si}}+\mathrm{O}_i \rightarrow I_{\mathrm{Si}}\mathrm{O}_i \text{ (not stable);}$$
$$I_{\mathrm{Si}}+\mathrm{O}_{2i} \rightarrow I_{\mathrm{Si}}\mathrm{O}_{2i} \text{ (stable);}$$

- **O-dimer bands (1012 and 1060 cm^{-1}) are suppressed;**
- **New bands (922 and 1037 cm^{-1}) are formed – shift with ^{18}O;**
- **DLTS give level $E_c - 0.1$ eV.**

Vibrational modes (cm^{-1})

	^{16}O	^{16}O-^{18}O	^{16}O-^{18}O	^{18}O
Obs	1037	ND	ND	46
	922	ND	ND	39
B	1020.7	44.9	0.3	45.8
	958.9	0.7	40.9	41.0
C	929.6	2.4	23.5	41.1
	898.7	37.1	17.3	39.2

Summary

- Growth kinetics of TDD(N) explained by rapid motion of oxygen chains (Murin, Markevich)
- Core consists of a pair of long oxygen chains linked to second Si neighbours
- Compression along [001] C_2 axis leads to empty strain induced gap band (SIB)
- Wavefunction of SIB localised on Si atoms – avoids oxygen
- Core has no donor activity
- Topological defects at ends of finite chain leads to double donor levels above SIB.

- **Donor electron transfer to SIB explains ENDOR results: observed shells are oxygen atoms lying near ends**

- **Magnitude and variation of piezospectroscopic tensors and LVMs consistent with experiment.**

- **Decreasing depth of SIB with N consistent with variation of donor level**

- **Passivation of ends of chains should leave acceptor activity due to SIB — evidence?**

- **$I\mathrm{O}_2$ is stable up to 300 K, with:**
  - **$(-/0)$ level at $E_c - 0.1$ eV;**
  - **$(0/+)$ level?**
  - **LVMs at 1037, 922 cm^{-1}.**