Oxygen-related defects in germanium

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Outline

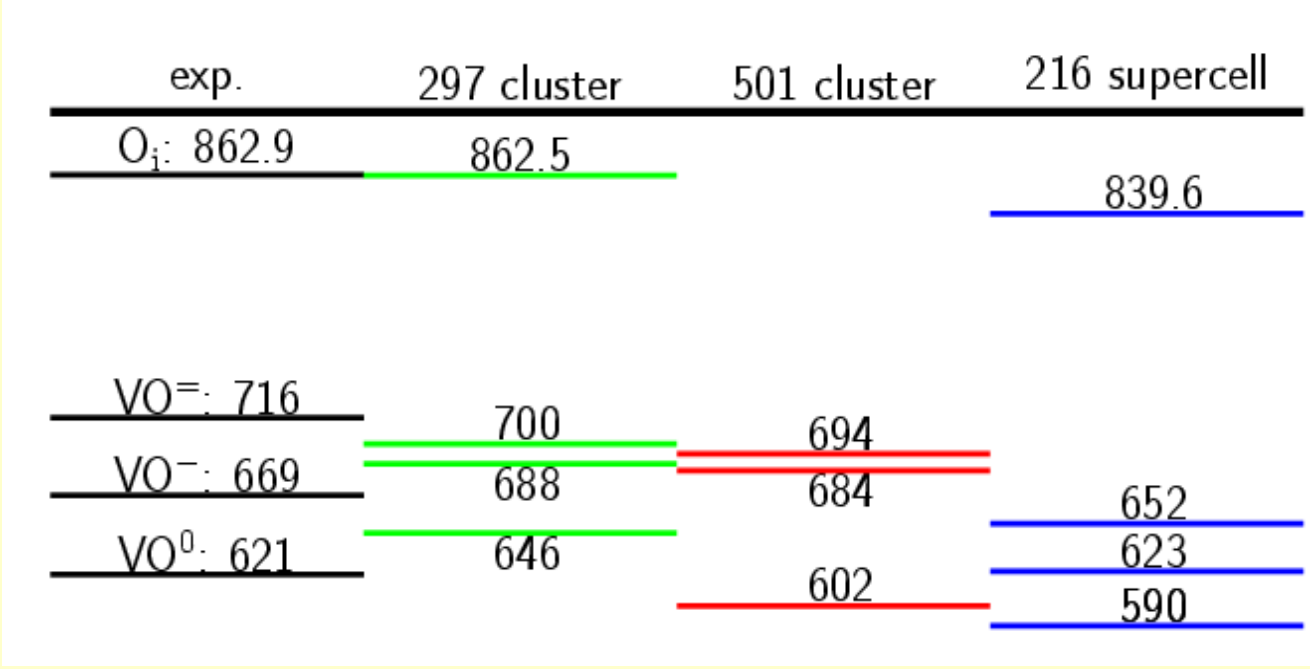
- VO
  - Electric levels and LVMs
  - Diffusion and dissociation
- Other V-O defects:VO*,VO_2,VO_2*,VO_2**
- IO_2

Method-general remarks

- Cluster: 297 or 501 atoms
  (the bandgap problem is avoided)
- Supercells of 216 atoms used for comparison
  (give lower bound for diffusion energies)
- Non-linear core correction (NLCC)
  (to account for the 3d semicore electrons)
- Diffusion barriers using the Nudged Elastic Band (NEB) method

VO

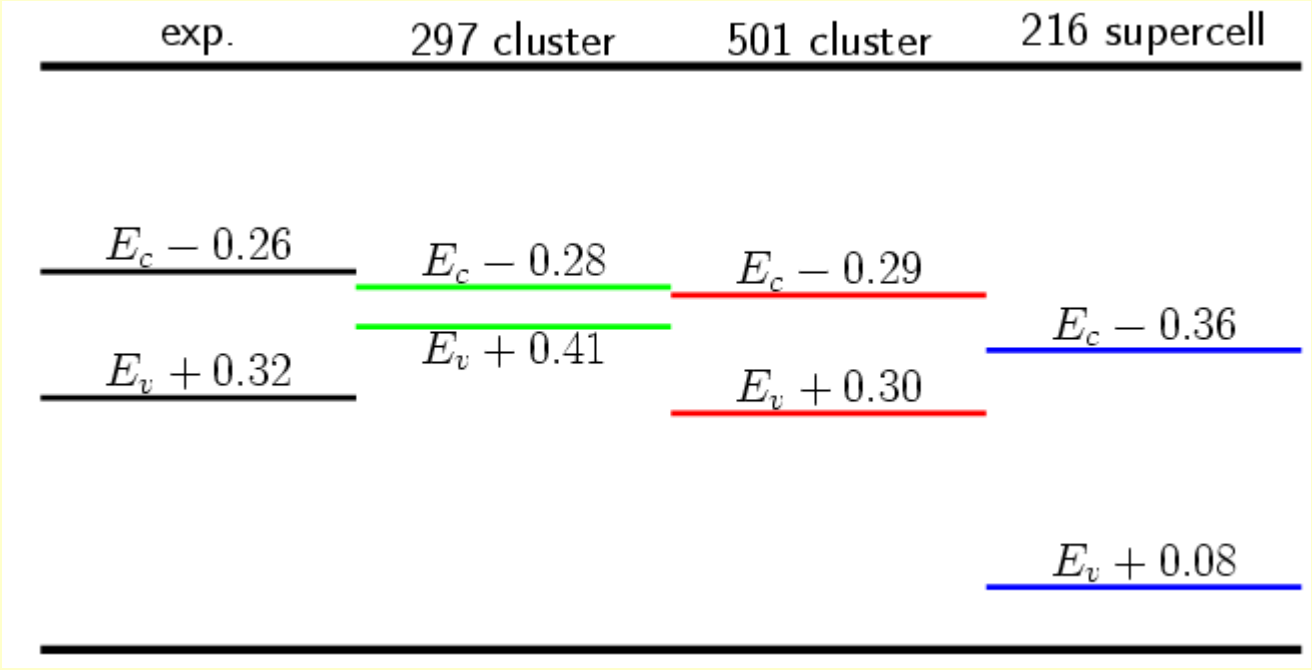
- LVMs predicted using both the cluster and supercell method



(frequencies in cm^{-1}, energies in eV, exper. from Markevich *et al.*)

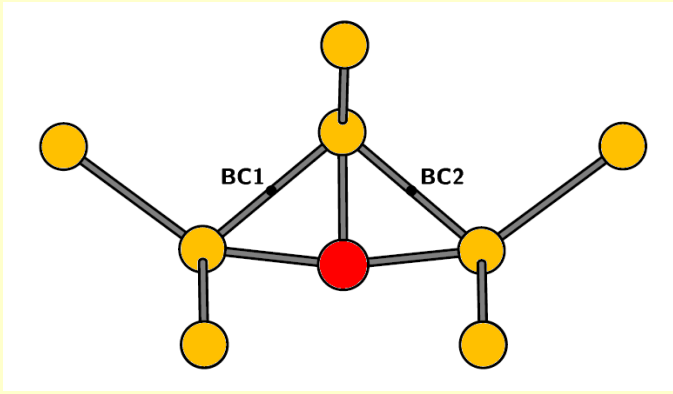
VO

- Electric levels in the supercell are no good: this will be reflected in calculated total energies



VO

- Test: hopping of O_i
  - supercell:1.42eV
  - cluster:2.35eV
  - exper. 2.08eV

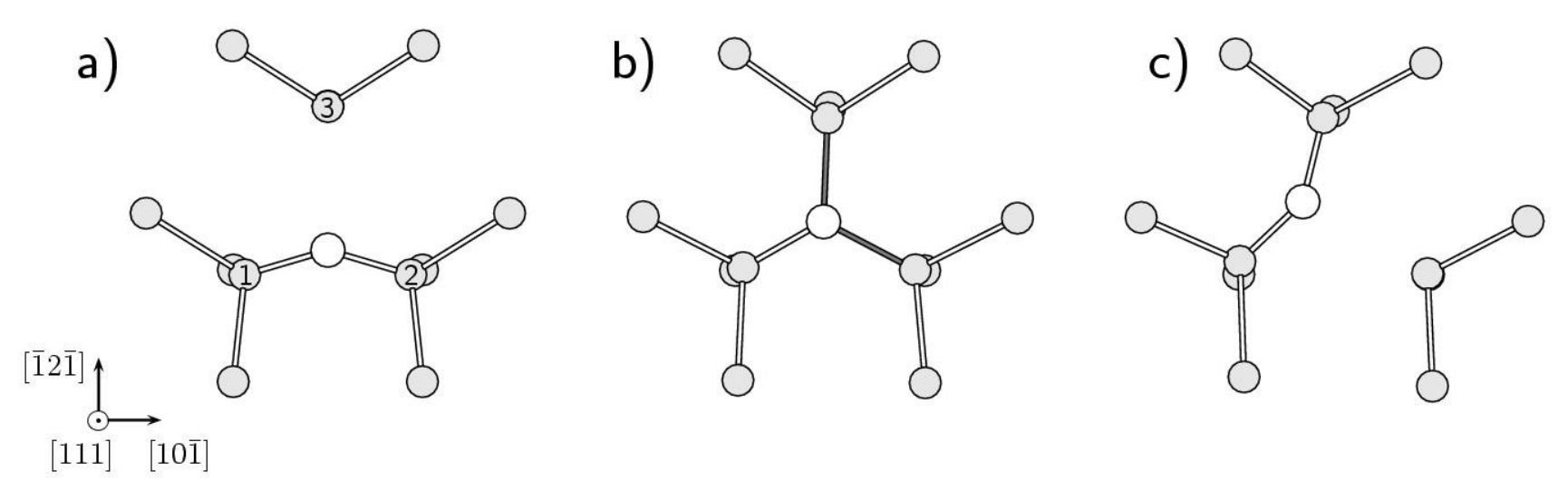


$E_{\text{barrier,sup}} > E_{\text{barrier,cluster}}$ may reflect the gap

- Main limitation of the cluster: calculation of binding energies (interaction with the surface)

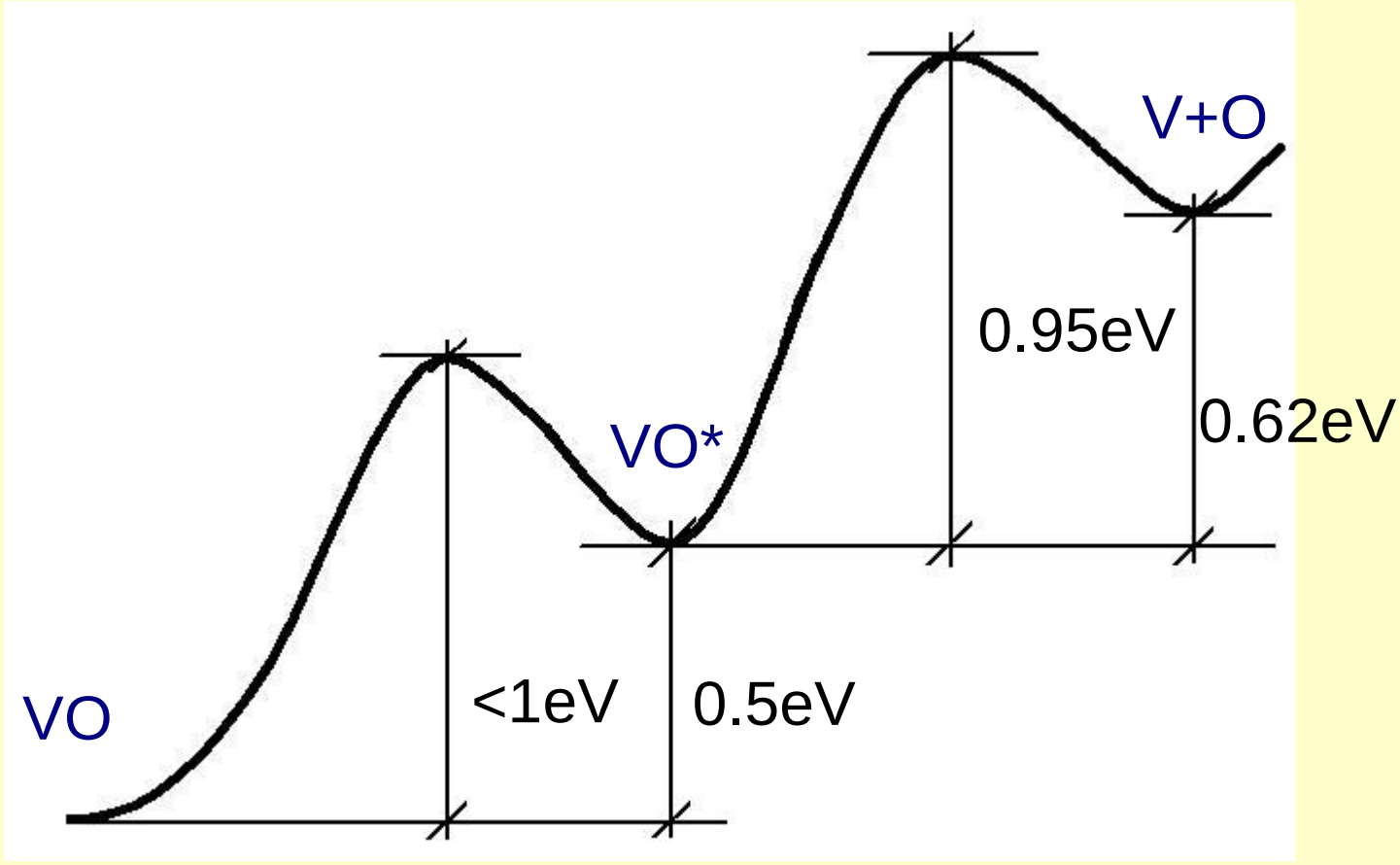
VO: reorientation

- **calc.:** reorientation barriers are found to be 0.11, 0.23 and 0.40 eV (501 atom clusters)
- **exper.**: no isotope splitting of 621 cm^{-1} band; No stress alignement of the (--/-) DLTS peak; No stress splitting of the (--/-) or (-/0) DLTS peaks;



VO^0: dissociation

Overall barrier:1.4eV



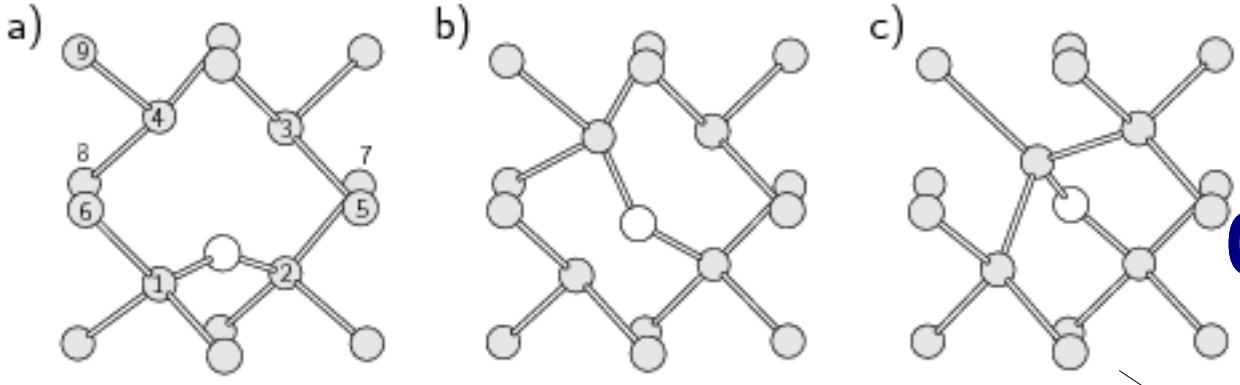
VO: dissociation and migration

migration

VO'

VO

VO*

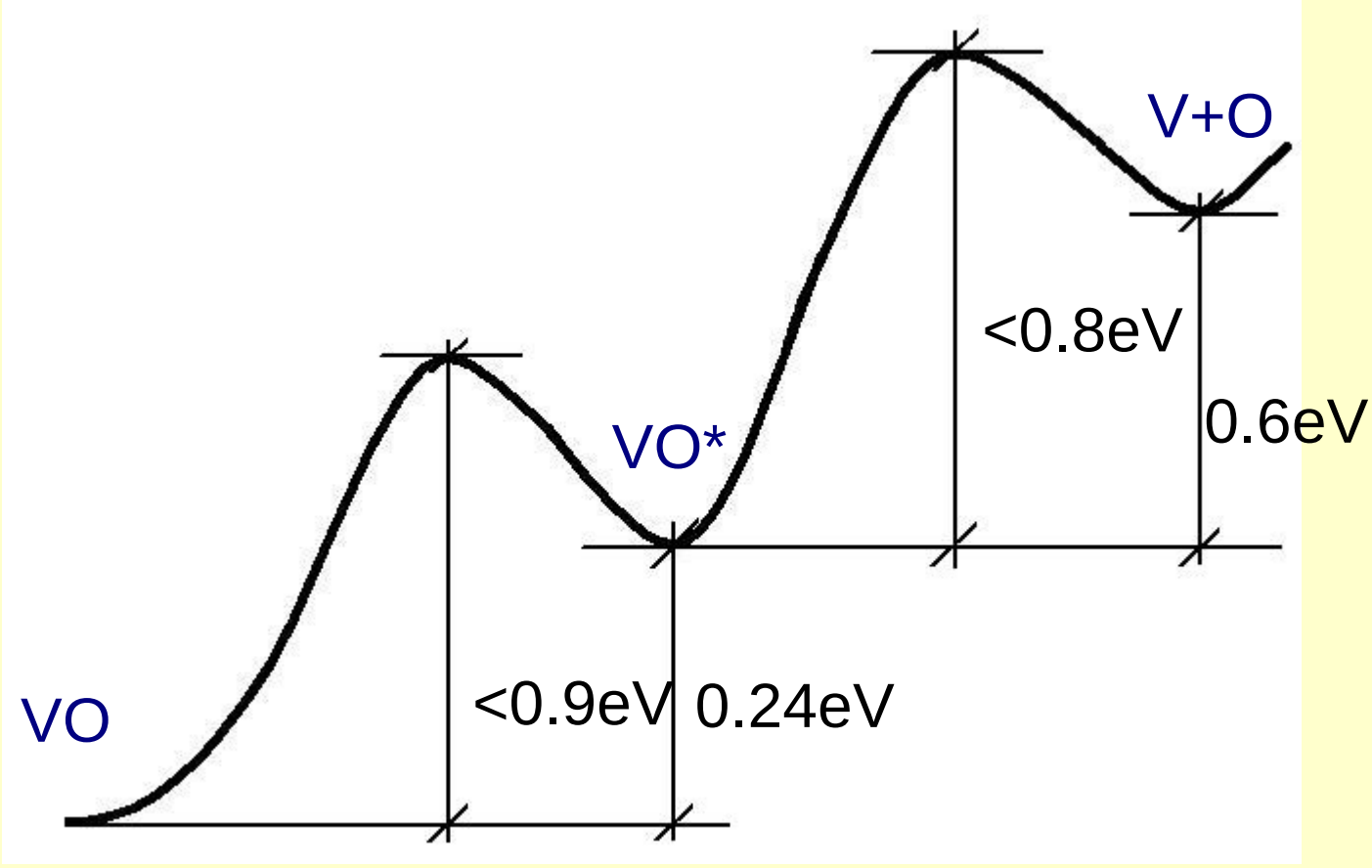


dissociation

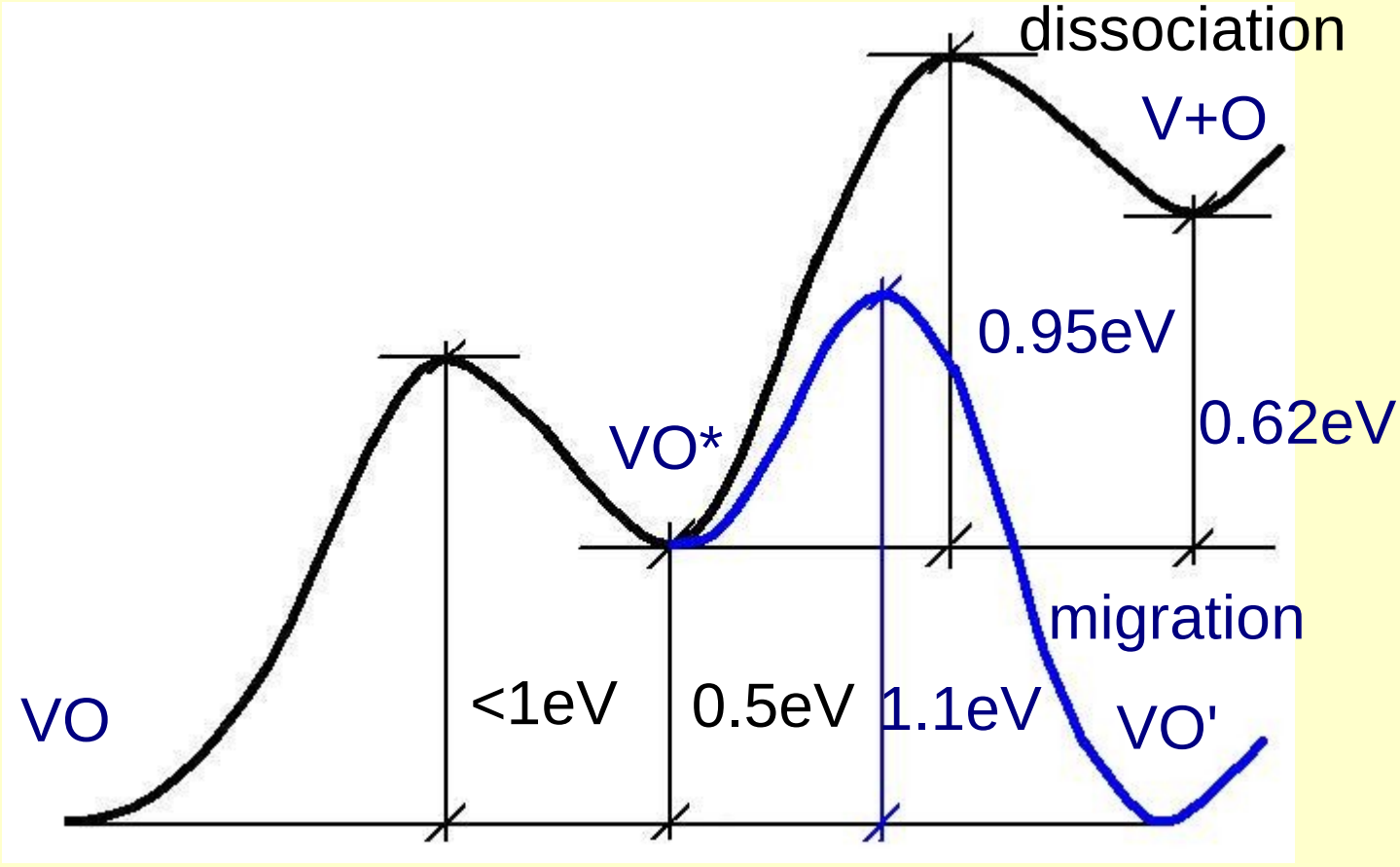
V+O

VO^-: dissociation

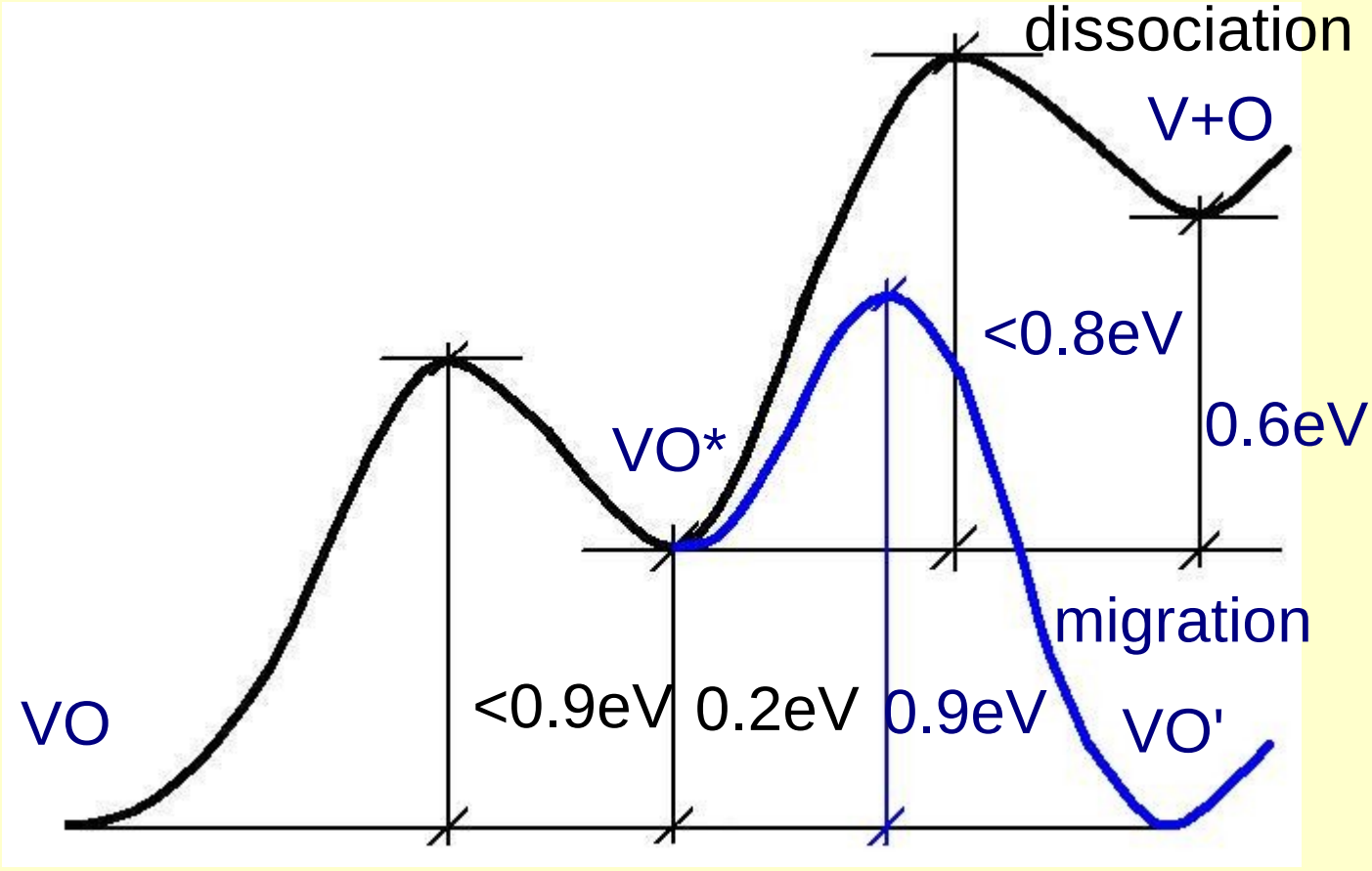
Overall barrier: <1 eV



VO^0: dissociation



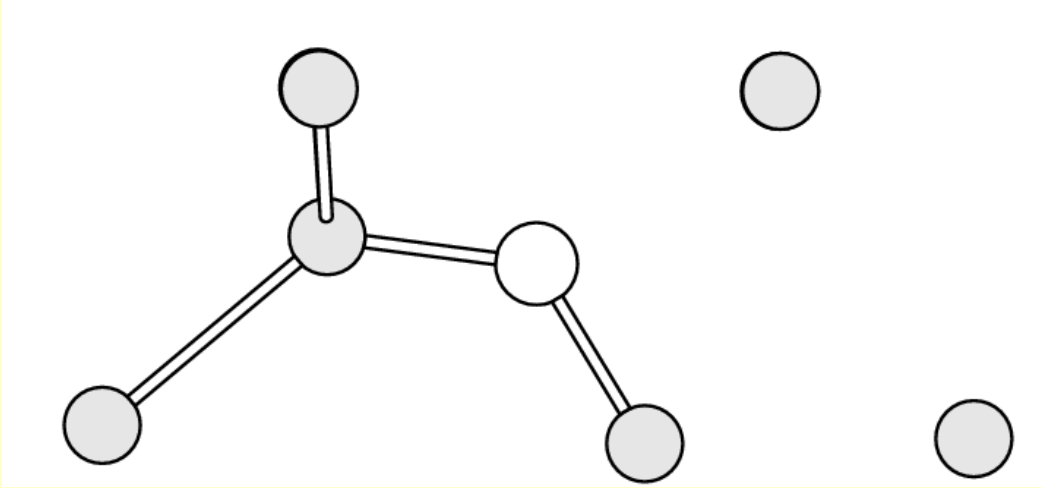
VO^-: dissociation



VO - dissociation or migration: linking with experiment

EXPERIMENT		INTERPRETATION?
• Annealing of VO(=/-) DLTS peak in Ge:Bi followed by a growth of BiV (Markevich *et al.*, 2006)	→	VO- dissociates?
• Annealing of VO levels in Hall effect measurements: activation energies and prefactors of 0.9eV and $10^{7}s^{-1}$ for VO^{-} (1.2eV and $10^{13}s^{-1}$for VO^{0}?) (Litvinov *et al.*,1984)	→	*v* suggest VO- migrates while VO^{0} dissociates?
• Possible formation of VO_2 after the annealing of VO (Litvinov, unp.)	→	suggesting migration of VO as a unit?

VO*: LVMs

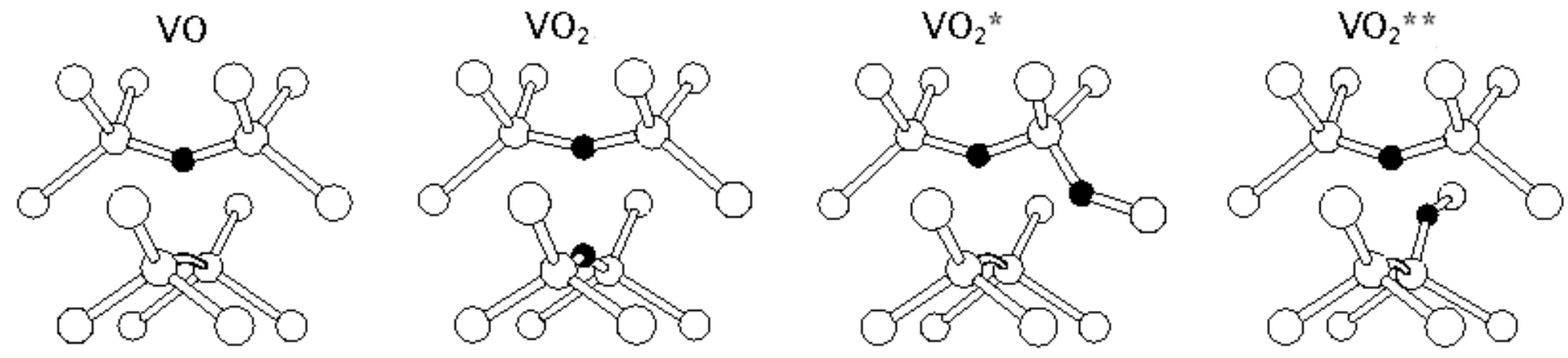


	VO^0	$VO^0(^{18}O)$	VO^-
297 cluster	704	667 (37)	720 (17)
216 supercell	708	672 (36)	718 (10)
Whan exp.	719	683 (36)	736 (17)

(all in cm^{-1})

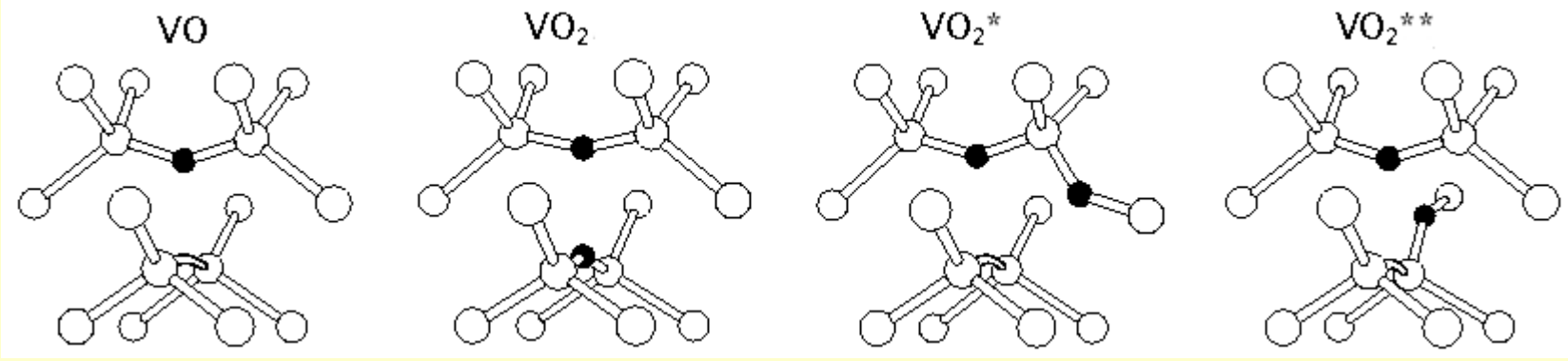
-/0 level at Ev+0.19 eV in a 297 atom cluster (Ev+0.29 eV supercell)

VO_2: Structures



VO_2: Energetics and electric levels (cluster)

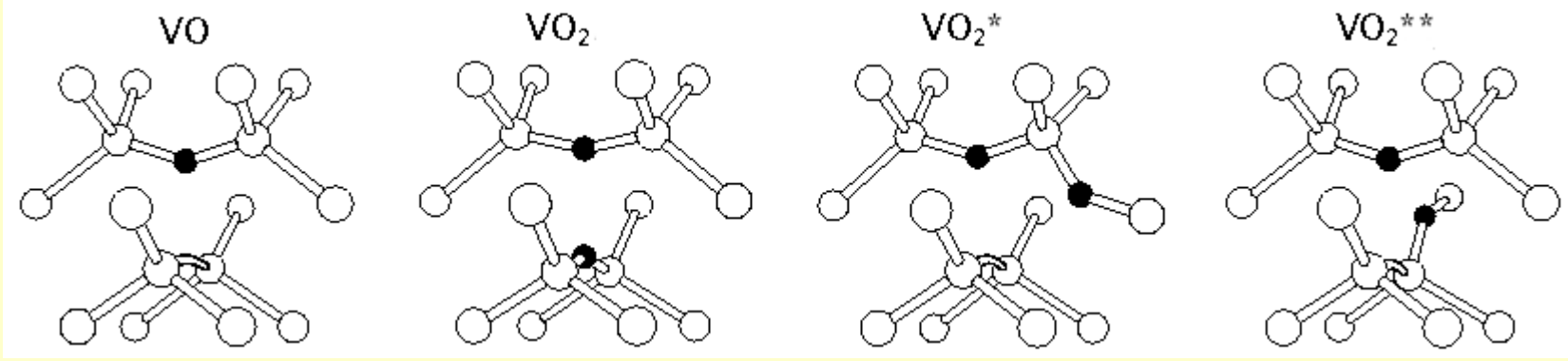
relative energy(eV)	VO_2	VO_2^*	VO_2^{**}
E_0	0.00	0.04	0.17
E_-	0.59	0.00	0.49



level -/0 at Ev+0.40eV

VO_2: LVMs (cluster)

VO_2^0	$VO_2^{*,0}$
707 (2x)	769
	682



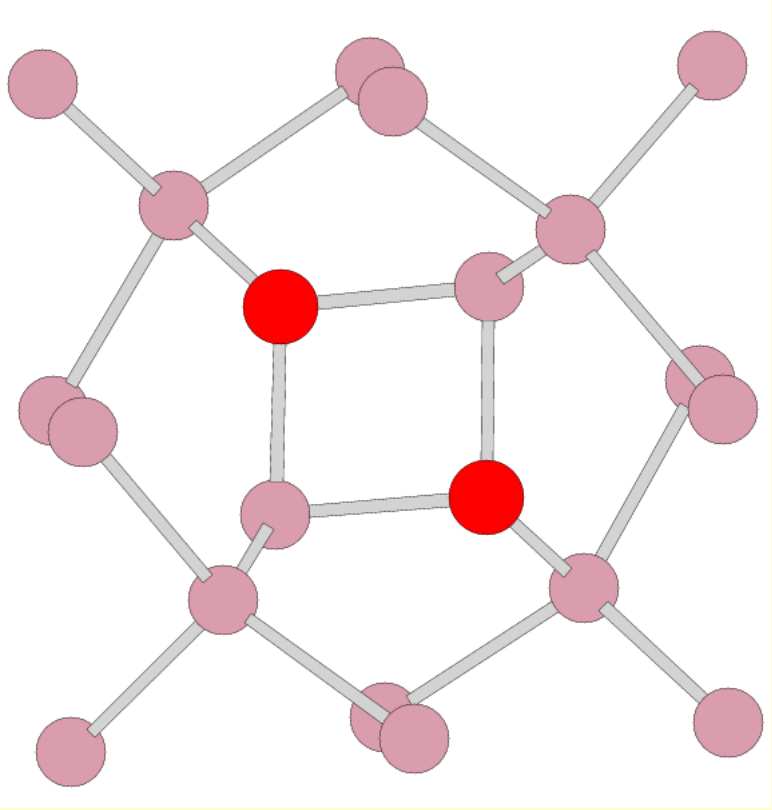
IO_2: Energetics and electric levels

relative energy (eV)	-	0	+	E (-/0)	E (0/+)
IO_2^A		0.91			
IO_2^B		0.68			
IO_2^C	0.64	0.72	0.83		
IO_2^E		1.11			
IO_2^F	**0.00**	**0.00**	**0.00**	Ev+0.93	Ev-0.19
IO_2^G	1.19	1.16	0.05?		

only one charge state

IO_2: Equilibrium structure

IO_2^F (C_{2v})



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