Positronium emission from various semiconductors

~Si, SiC, GaN and AlN~

(i)Background, Why Ps from semicond.?
(ii)Methods, Experiment & Calculation
(iii)Ps TOF energy spectra
(vi)Summary & Future prospects

A. Miyashita	(QST)	Ab initio calculation
M. Maekawa	(QST)	Monte Carlo simulation
K. Wada	(KEK)	Ps-TOF measurement
Y. Nagashima	(Tokyo U. Sci.)	Ps-TOF instrumentation
A. Ishida	(Tokyo U.)	Multi-hit data processing
A. Kawasuso	(QST)	Designing research plan

Background

Why now investigation of Ps formation mechanism?

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"Ps＝Purely leptonic bound system"

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Bose-Einstein condensation
Atomic & Molecular Physics

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Ps Technologies
Mass generation & Manipulation

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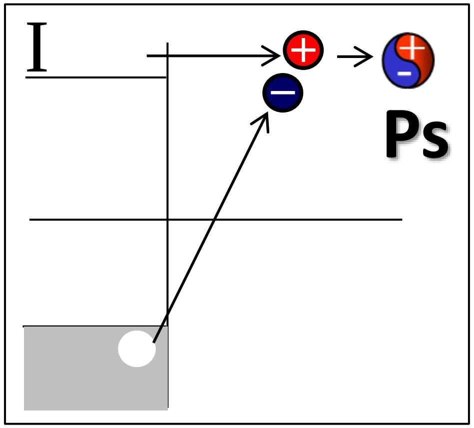
Details of Ps formation mechanism

Background



Direct Positronium Emission (Formation potential mechanism)

$\Phi_{Ps}=\Phi_{+}+\Phi_{-}-6.8eV<0$

$0 < E_{Ps}=-\Phi_{Ps}-E_F+E < |\Phi_{Ps}|$ E: Electron energy level

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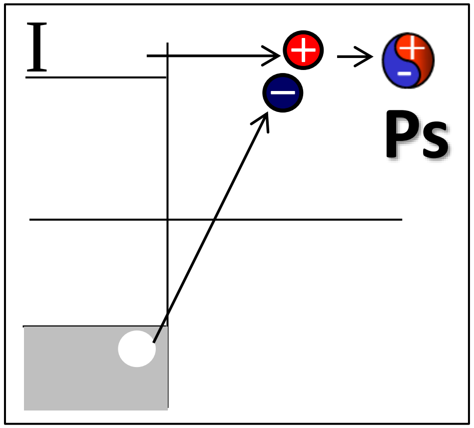

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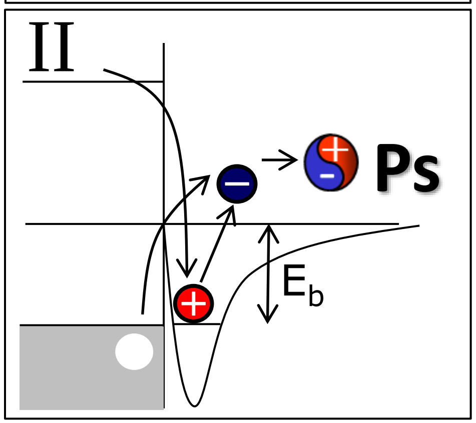

Surface Positron-mediated Emission

Thermal activation

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Athermal emission

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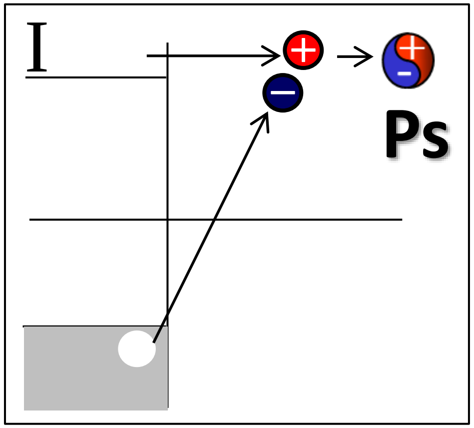

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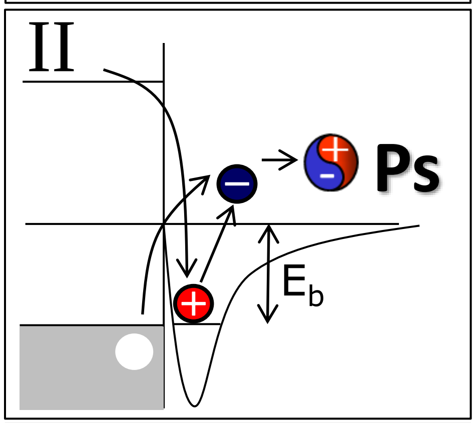

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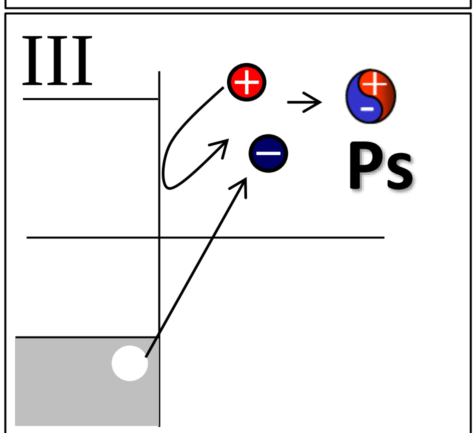

Dynamical neutralization process (LEPD scattering)

$$E_{Ps} \sim E_{+}- \Phi_{-} -E_{inelastic}+6.8eV$$

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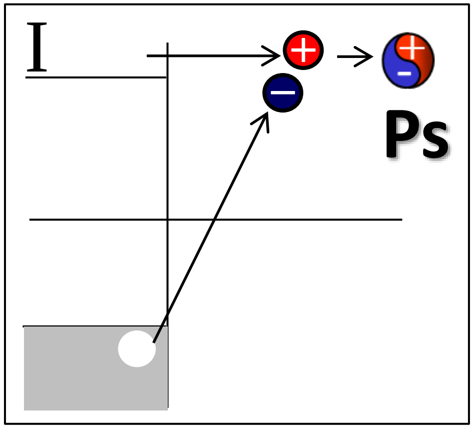

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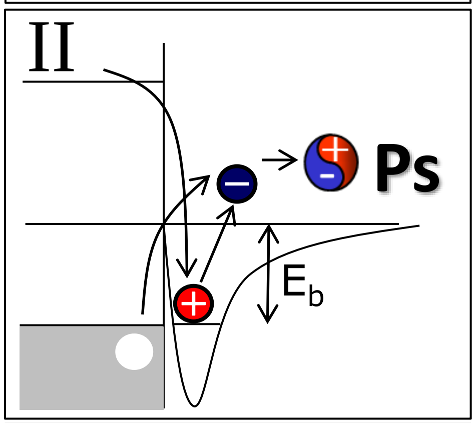

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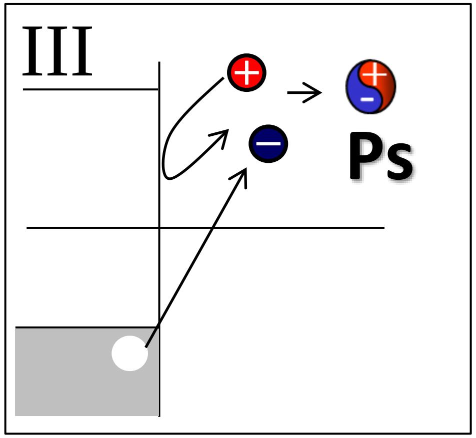
Independent of Ps formation potential



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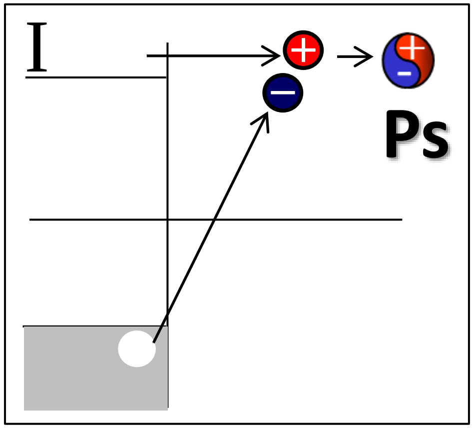

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$\Phi_{Ps} = \Phi_{+} + \Phi_{-} - 6.8\text{eV} < 0$

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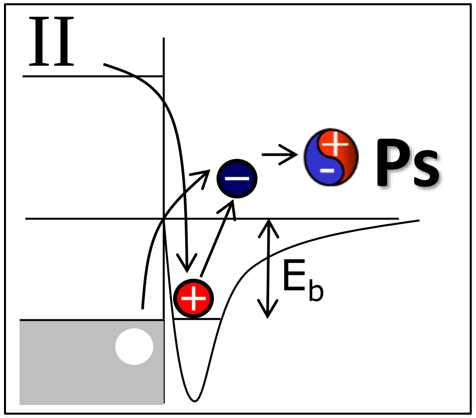

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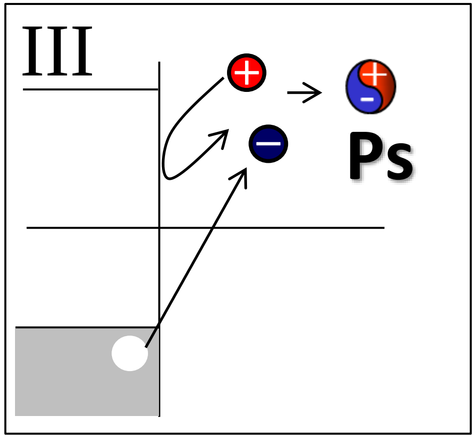

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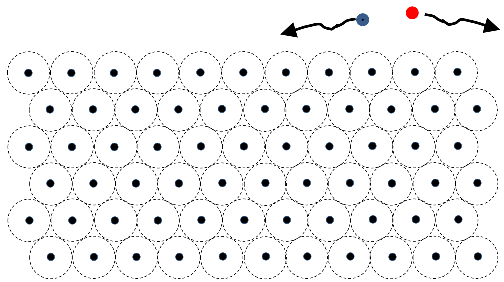
$E_{Ps} \sim E_{+} - \Phi_{-} - E_{inelastic} + 6.8\text{eV}$

Ps is easily formed at solid surfaces due to its various formation channels

Background

A scale image for Ps stability

Transition metals r_s~1



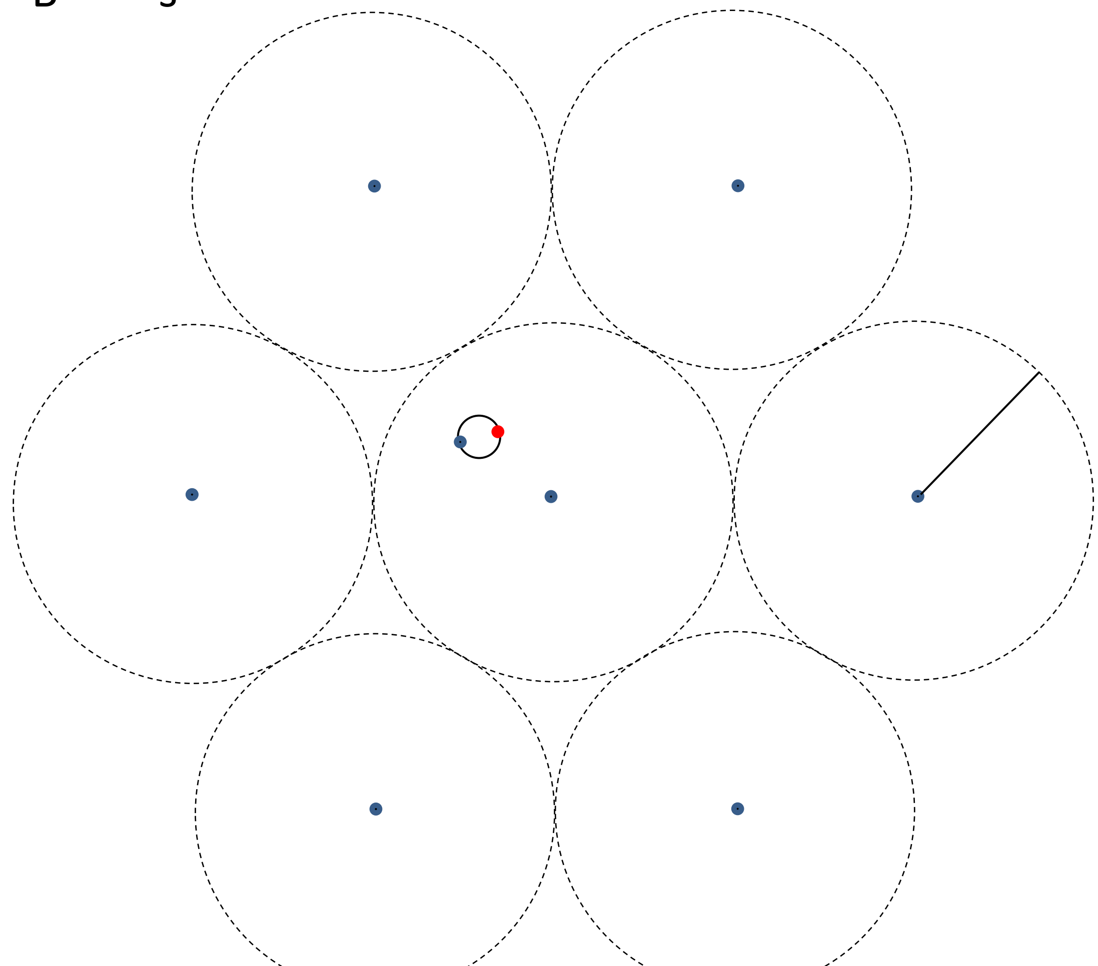
Electron

Ps

$r_{Ps}=a_B=1r_s$

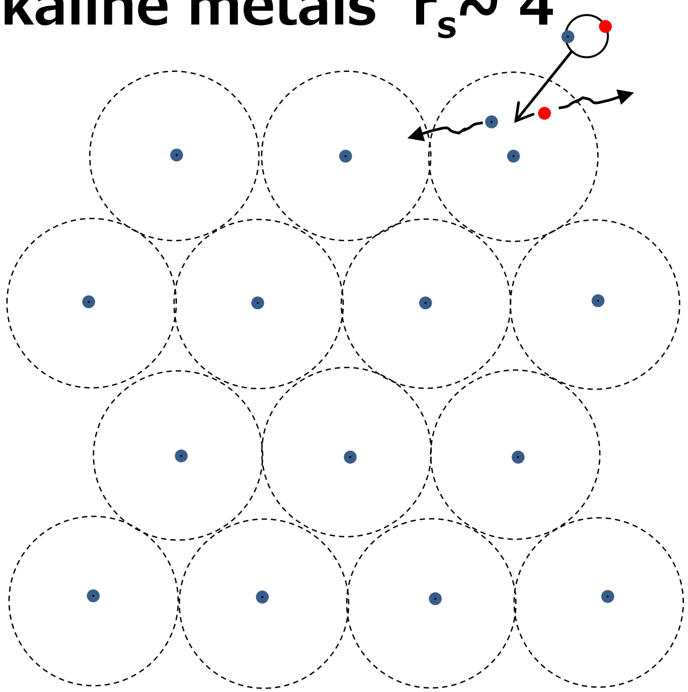
$$U(r)=\frac{e^2\exp(-\mu r)}{r}$$

$r_s = 8.5$ **Ps is formed**



Ps is prohibited

Alkaline metals r_s~ 4



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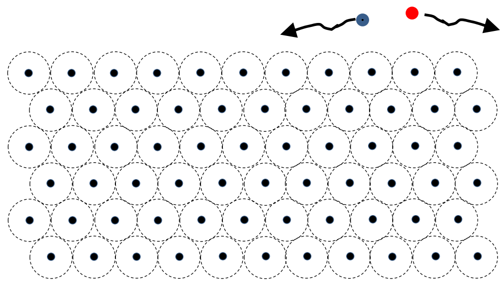

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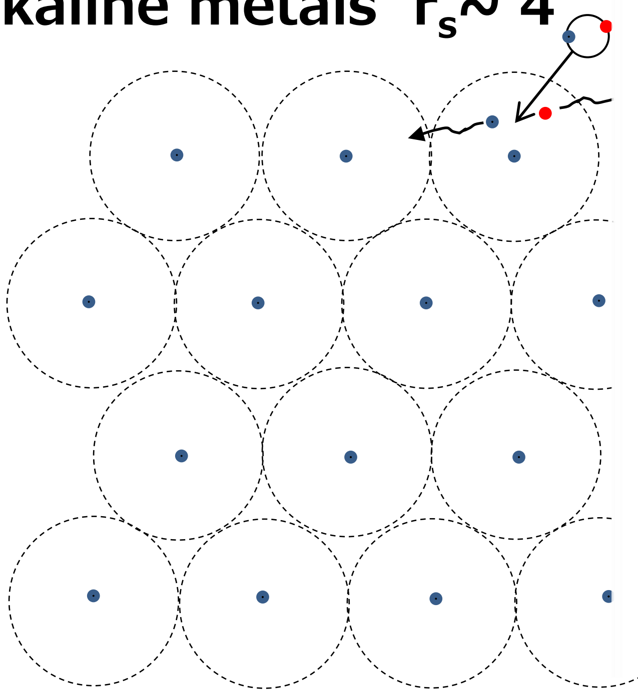
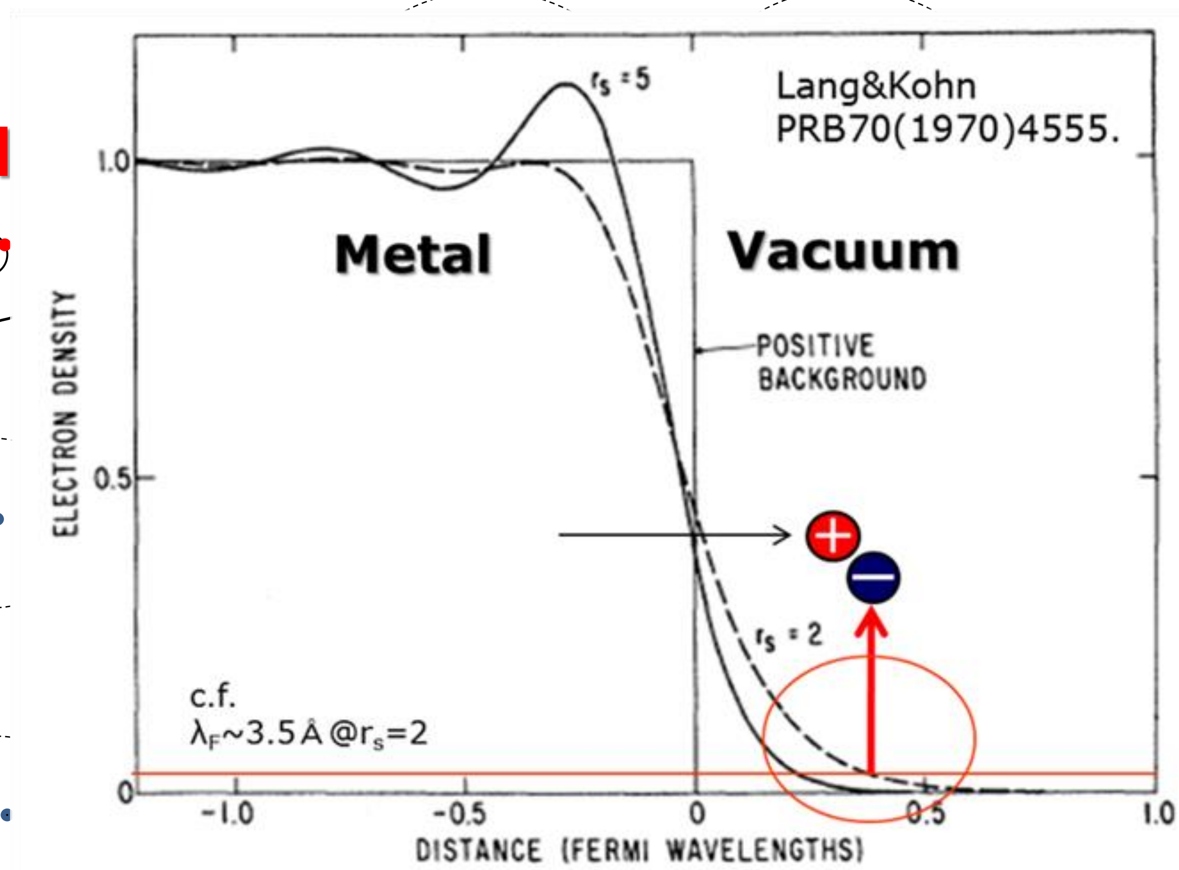
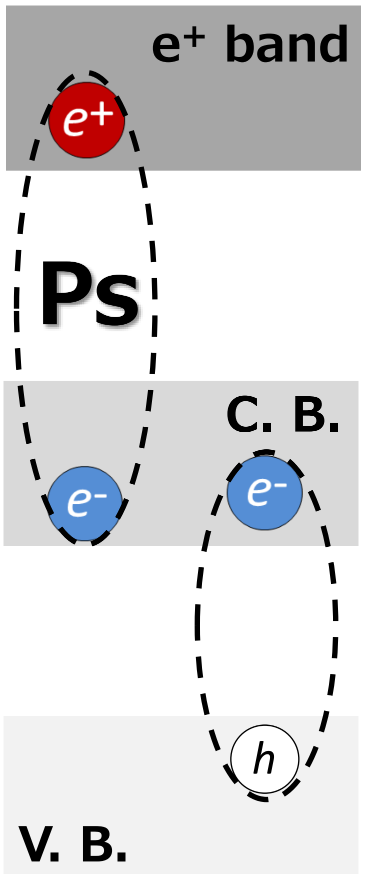
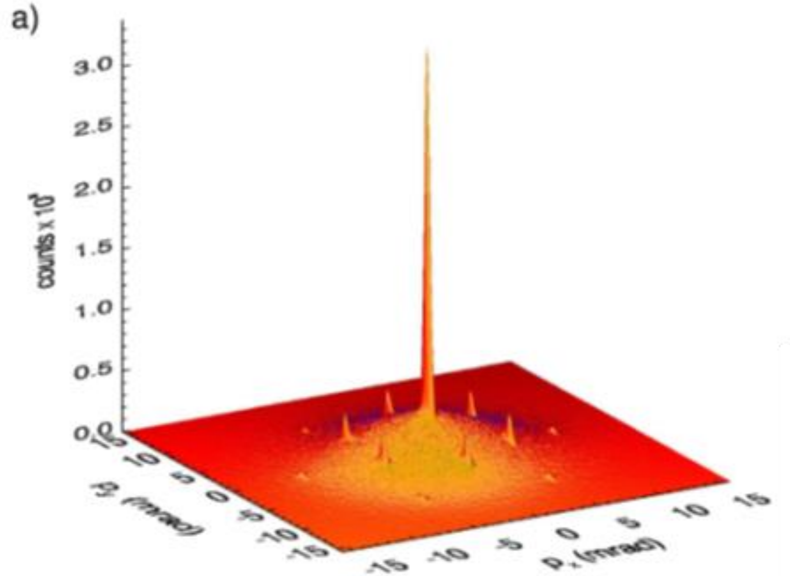




Ps formation in insulators

Wannier-Mott exciton
like Positronium





S B Dugdale *et al* 2013 *J. Phys.: Conf. Ser.* **443** 012083

Metal：Electron screening

$$U(r) = \frac{e^2 \exp(-\mu r)}{r}$$

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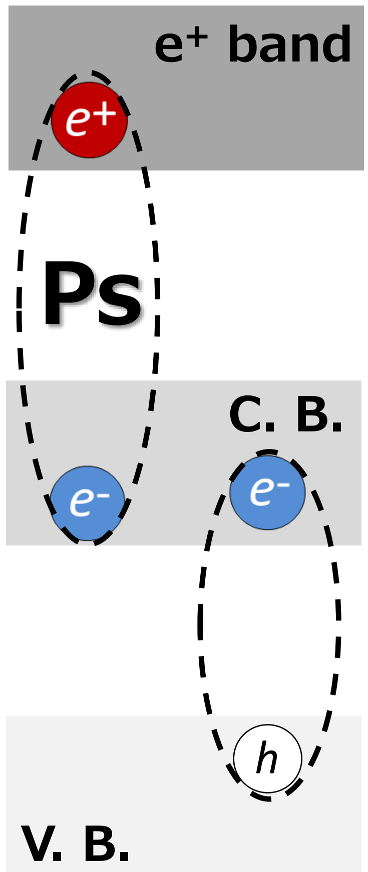

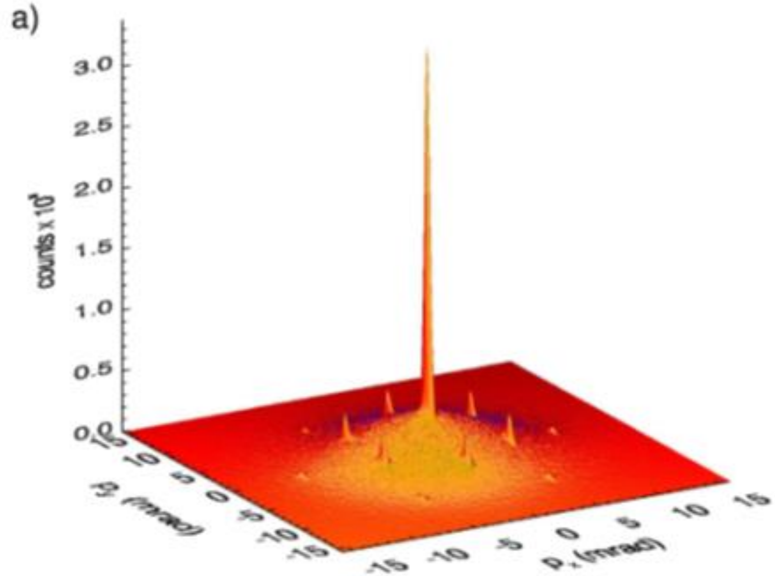

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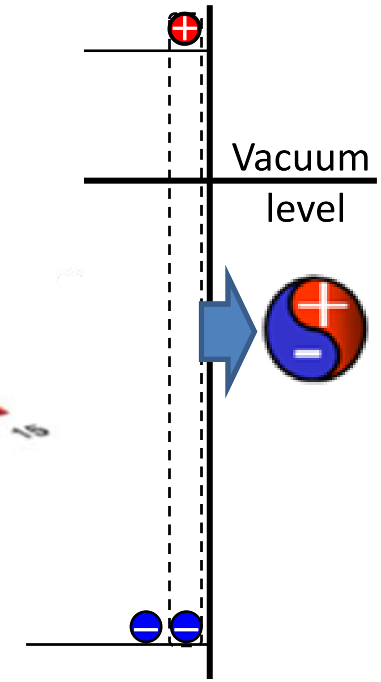

Ps emission inside to vacuum

Y. Nagashima et. al., PRB58(1998)12676

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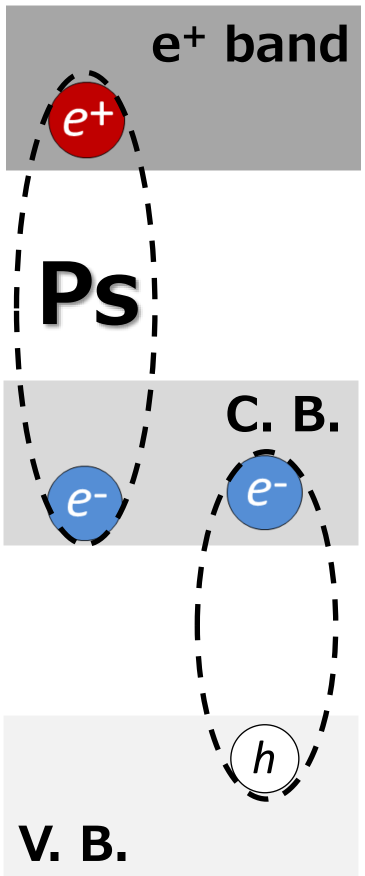

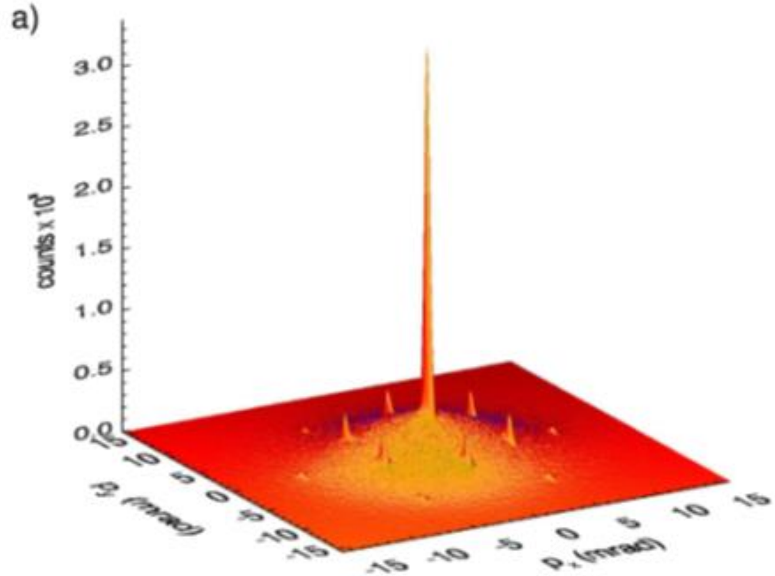

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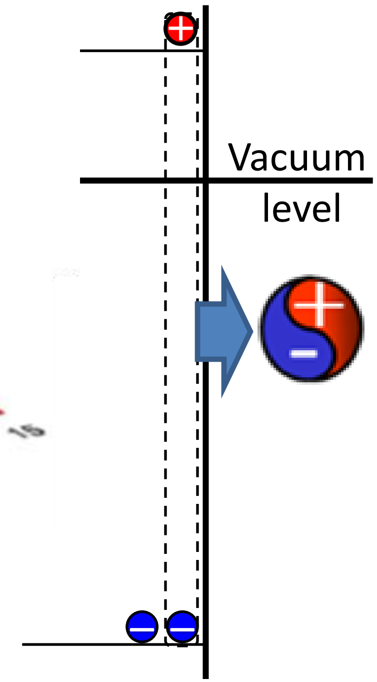

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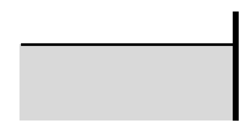

Emission of **e⁺** and **e⁻** as **Ps** ⇨ Formation potential (Neg.)

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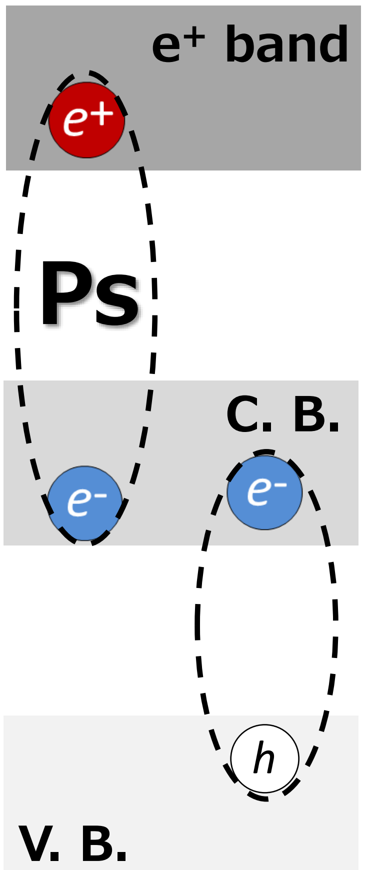

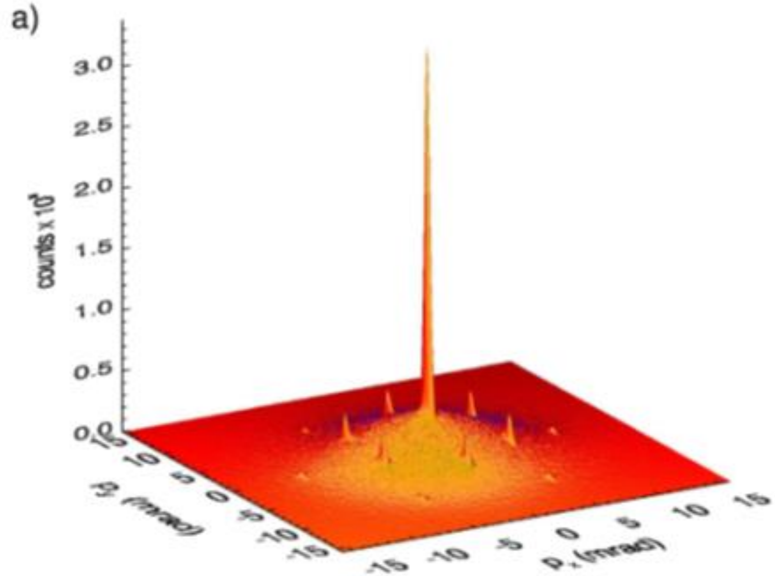

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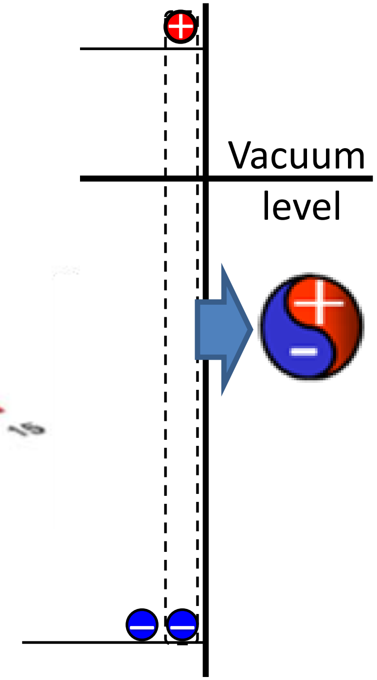

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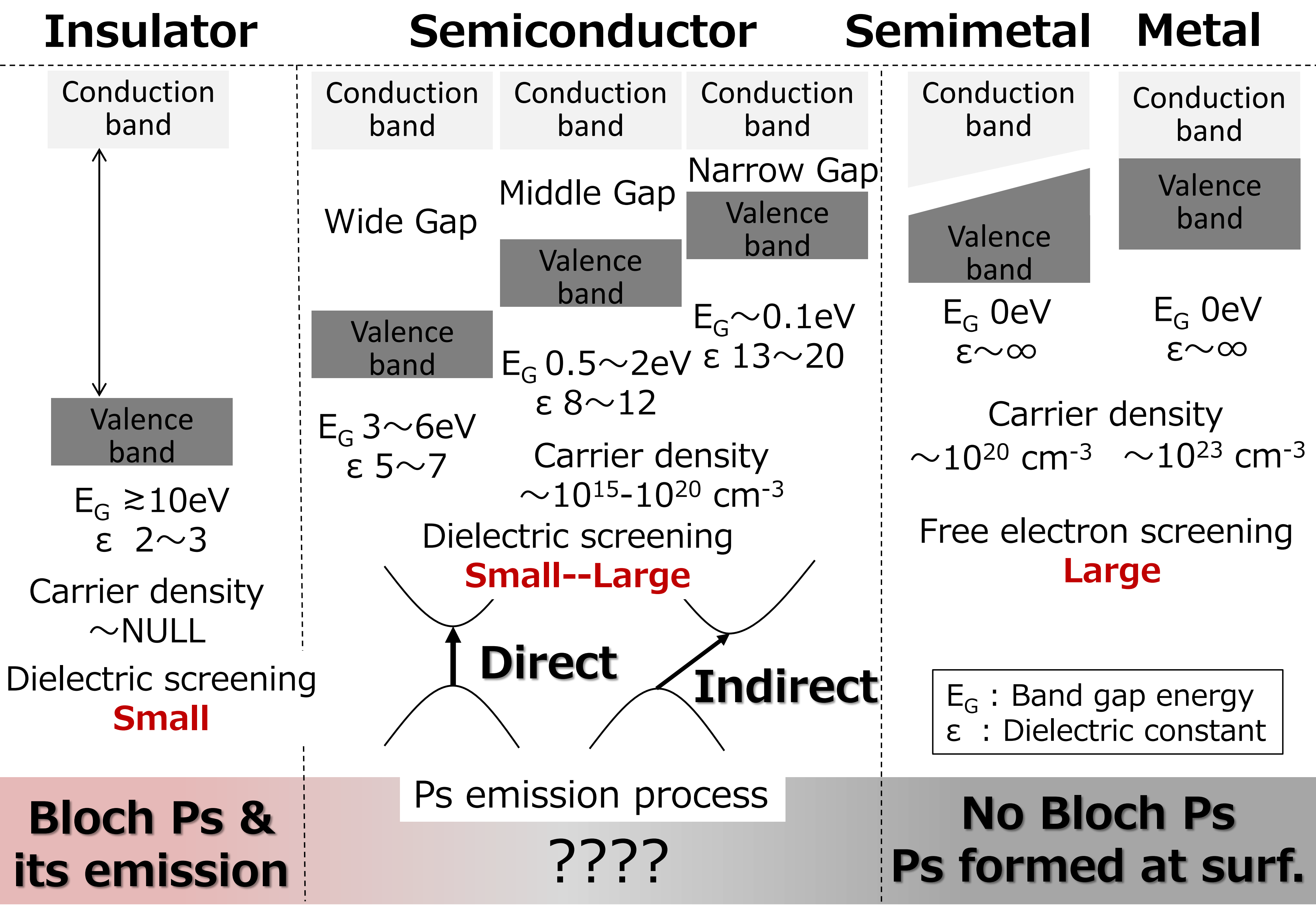
Emission of **Bloch Ps** ➡ Work function (Neg.)

P. J. Schultz&K. Lynn, RMP60(1988)701.

Material classification by conductivity and Ps formation



Expected characteristics?

Insulator・・・ Semiconductor ・・・Metal

Ps Bloch state・・・Yes in principle, hardly visible

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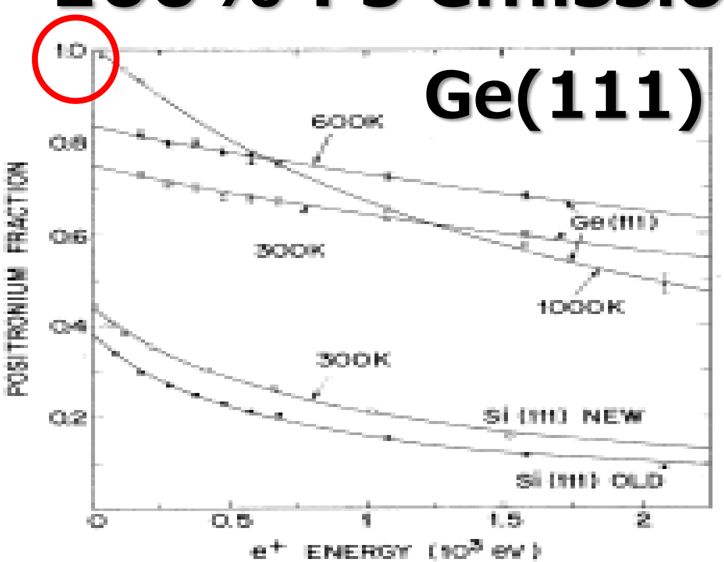

Mills PRL41(1978)1828-1831.

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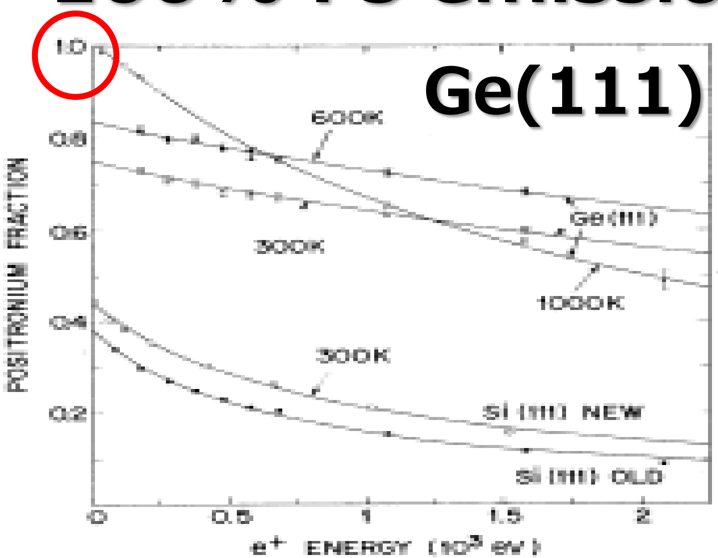

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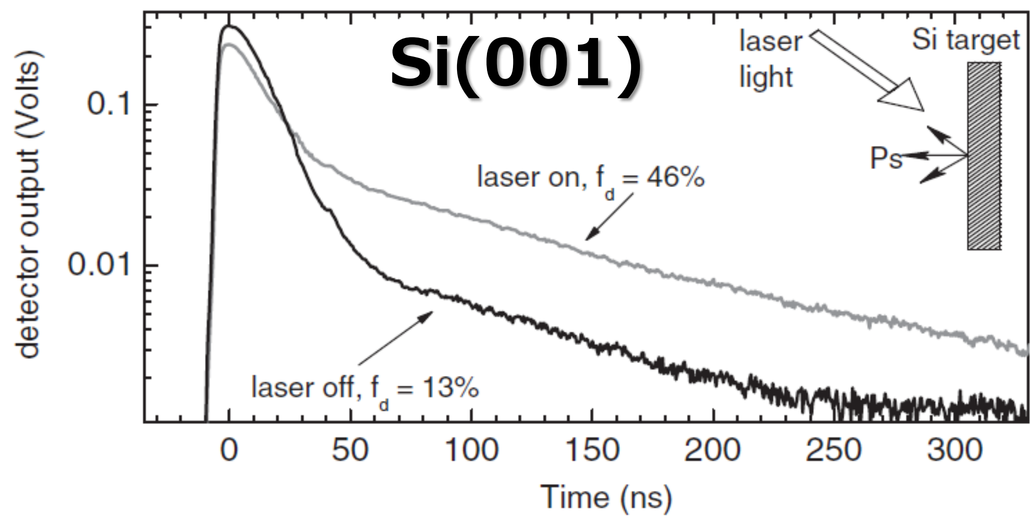
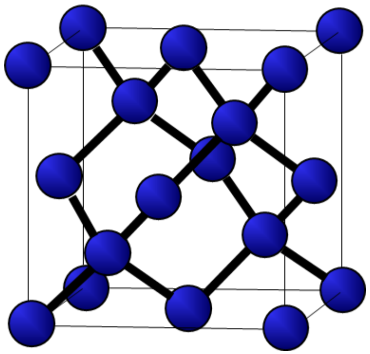
Photoemission of Ps

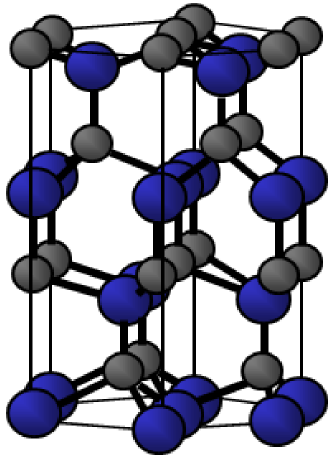


Cassidy, PRL107(2011)033401.

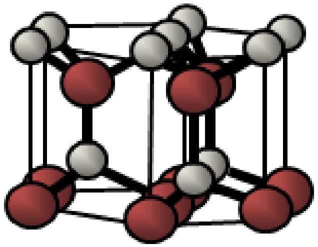
Parameter-free GGA calculation



Si



SiC



GaN, AlN

	Bulk calculation		Slab calculation			
	A_+	Φ_{Ps}	Surface	φ_-	φ_+	E_B
Si	-6.38eV	**-0.42eV**	(111)	+4.56eV	**+1.82eV**	**+2.70eV**
			(001)	+4.54eV	**+1.84eV**	**+2.41eV**
4H SiC	-4.71eV	**-2.10eV**	(0001)	+6.44eV	**-1.74eV**	**+2.24eV**
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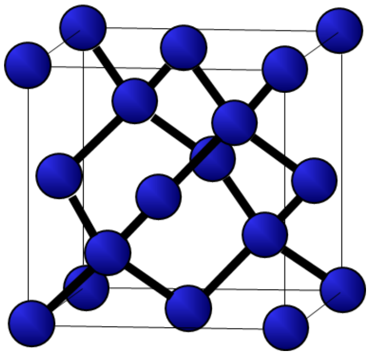

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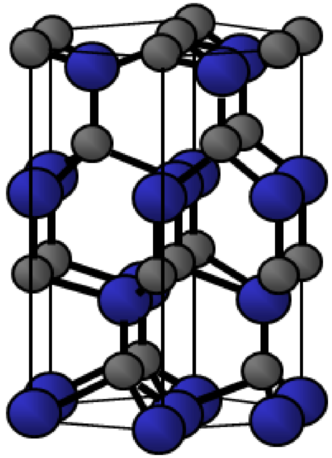

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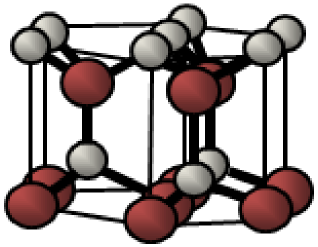

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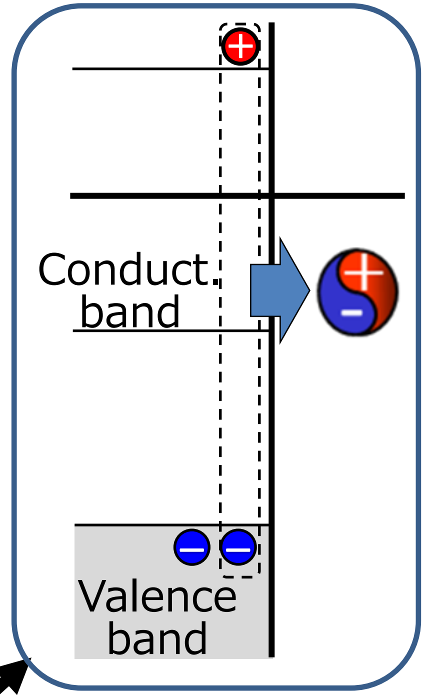

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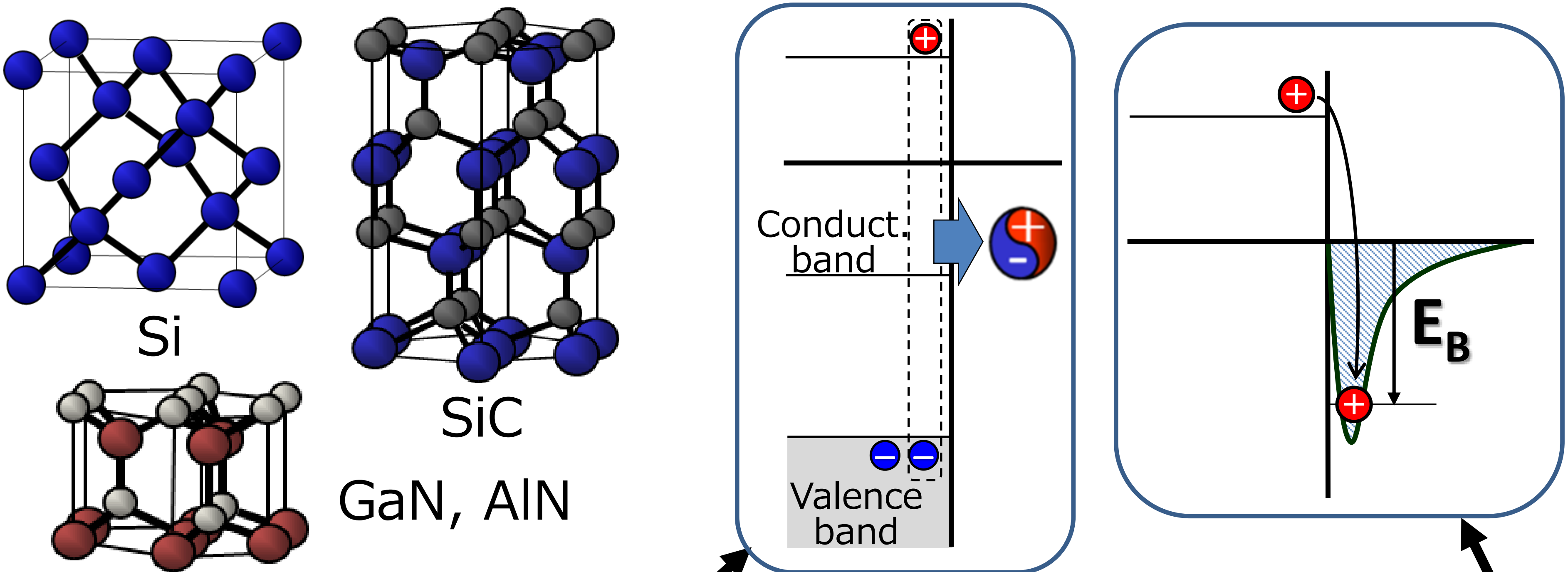

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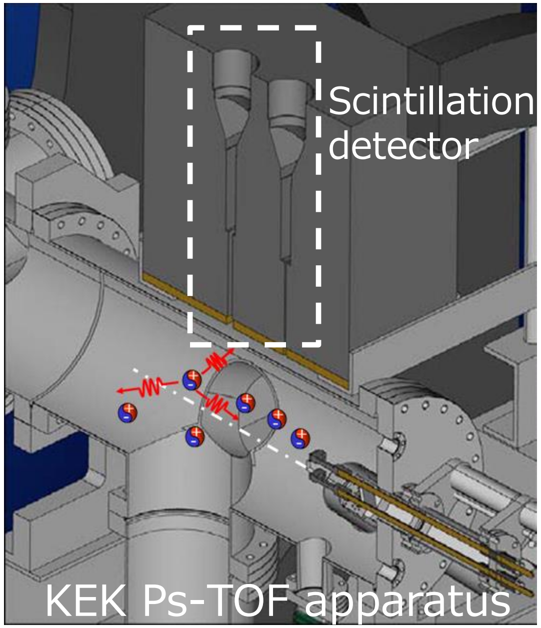
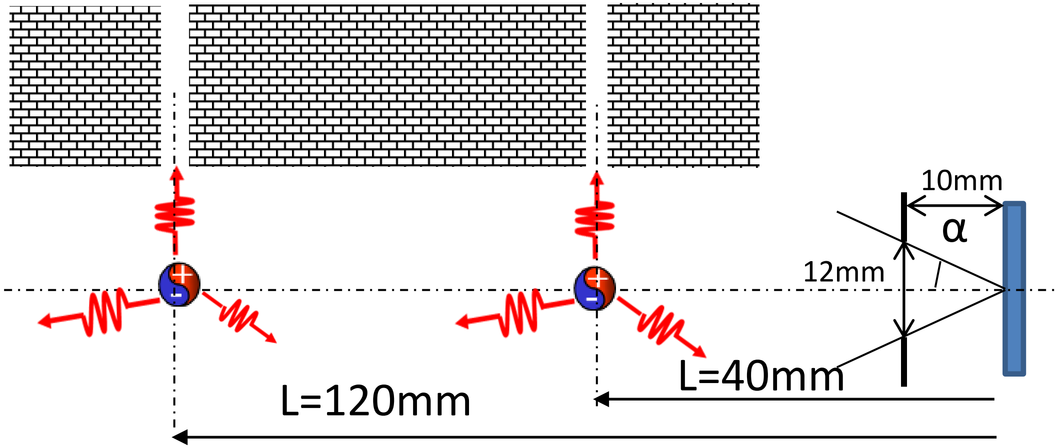
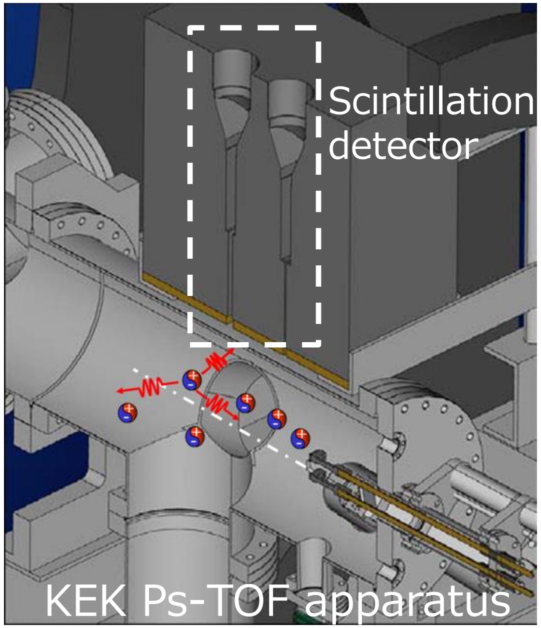
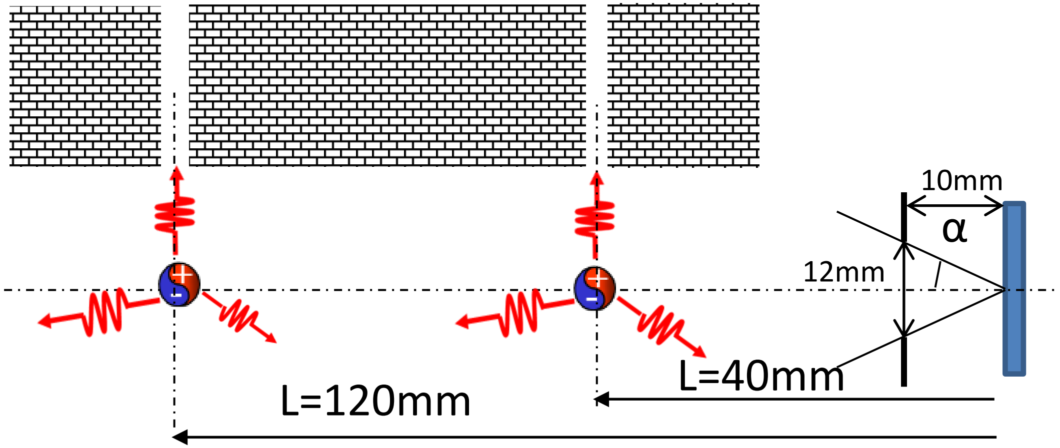
Experiment


Scintillation
detector
KEK Ps-TOF apparatus


10mm
α
12mm
L=40mm
L=120mm

Experiment



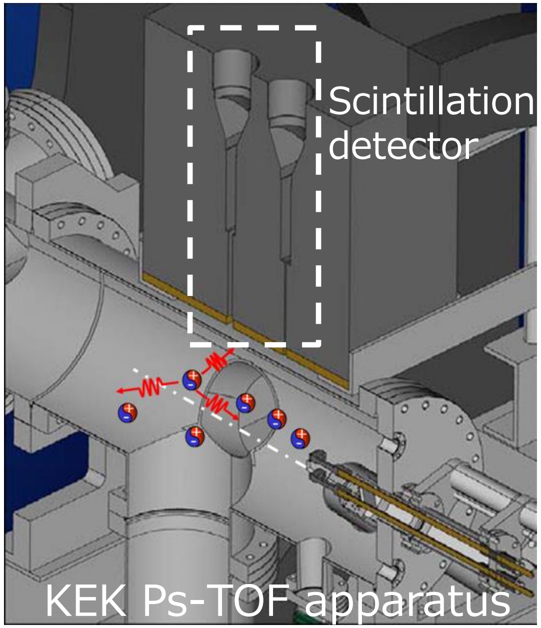


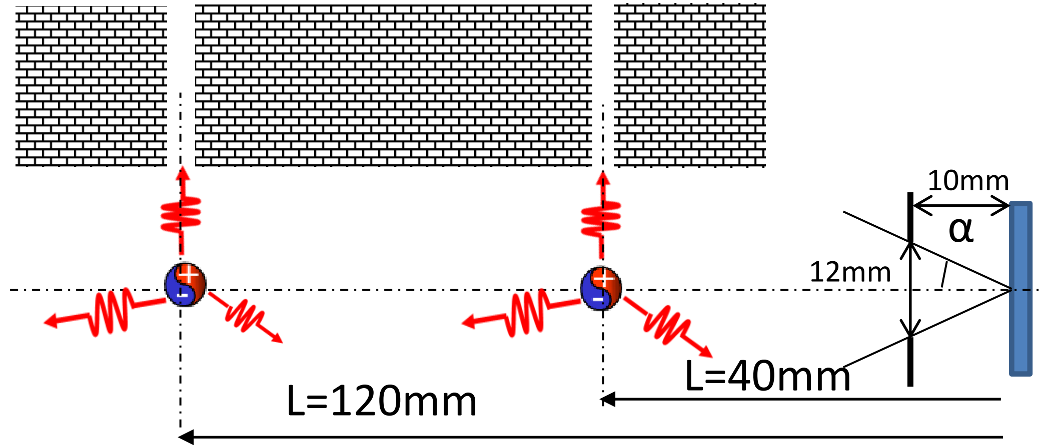
$$\frac{dN(E_\perp)}{dE_\perp} \propto t^2 \exp(t/142) N_{TOF}(t)$$

Energy Spectrum

TOF Spectrum

Experiment





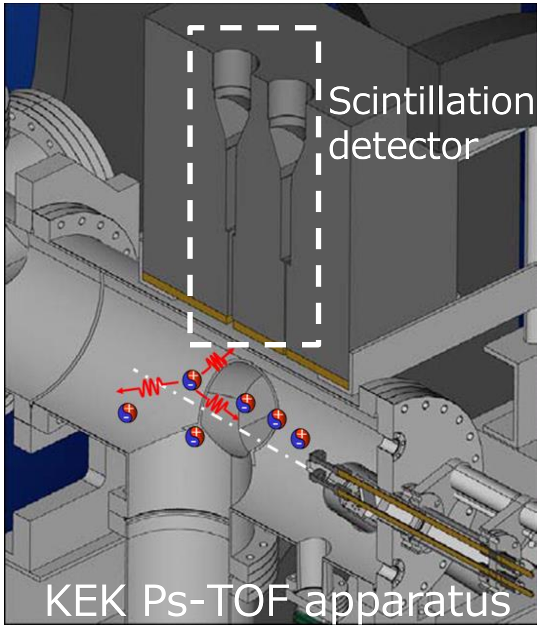
$$\frac{dN(E_\perp)}{dE_\perp} \propto t^2 \exp(t/142)\, N_{TOF}(t)$$

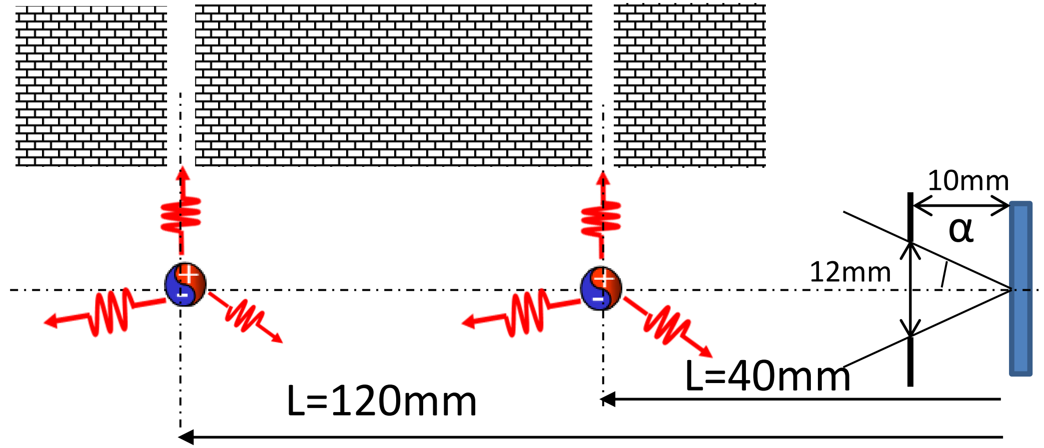
$\frac{dN(E_\perp)}{dE_\perp}$: Energy Spectrum

$N_{TOF}(t)$: TOF Spectrum

$$t = L\sqrt{m/E} \qquad N_{TOF}(t) \rightarrow N_{TOF}(E)$$

Experiment





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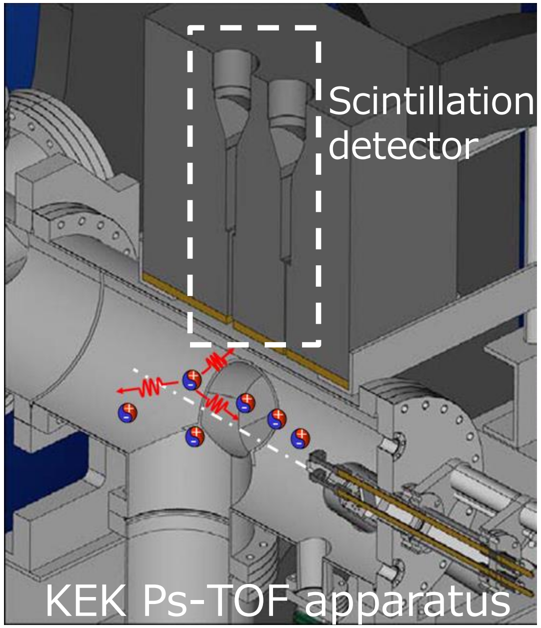
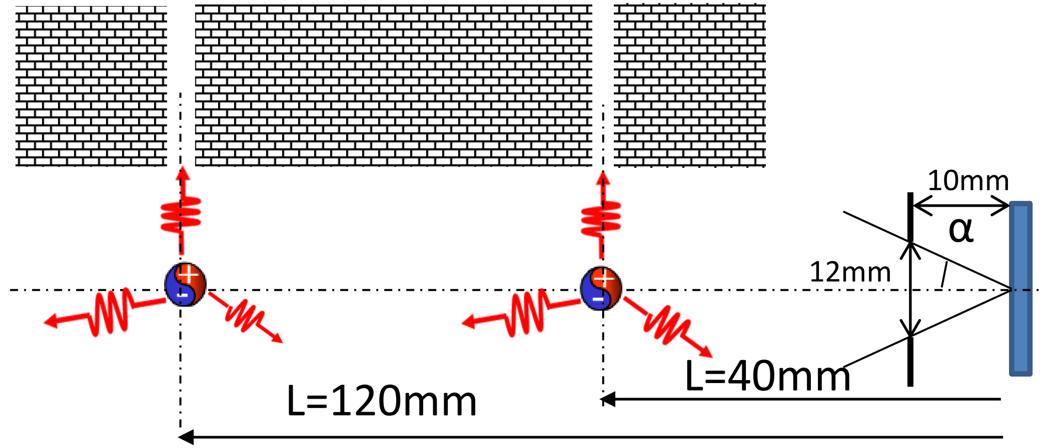
Energy Spectrum — TOF Spectrum

$$t = L\sqrt{m/E} \qquad N_{TOF}(t) \rightarrow N_{TOF}(E)$$

Material	Characteristics	Treatment
Si(111)	**Sb-dope (n:1x10^{18}cm^{-3})**	**HF & UPW cleaning**
4H SiC(0001)	**N-dope (n:10^{17}cm^{-3})**	**HF & UPW cleaning**
***h* GaN(0001)**	**Undope (n-type)**	**Ethanol cleaning**
***h* AlN(0001)**	**Undope**	**Ethanol cleaning**

Experiment





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$\frac{dN(E_{\perp})}{dE_{\perp}}$: Energy Spectrum

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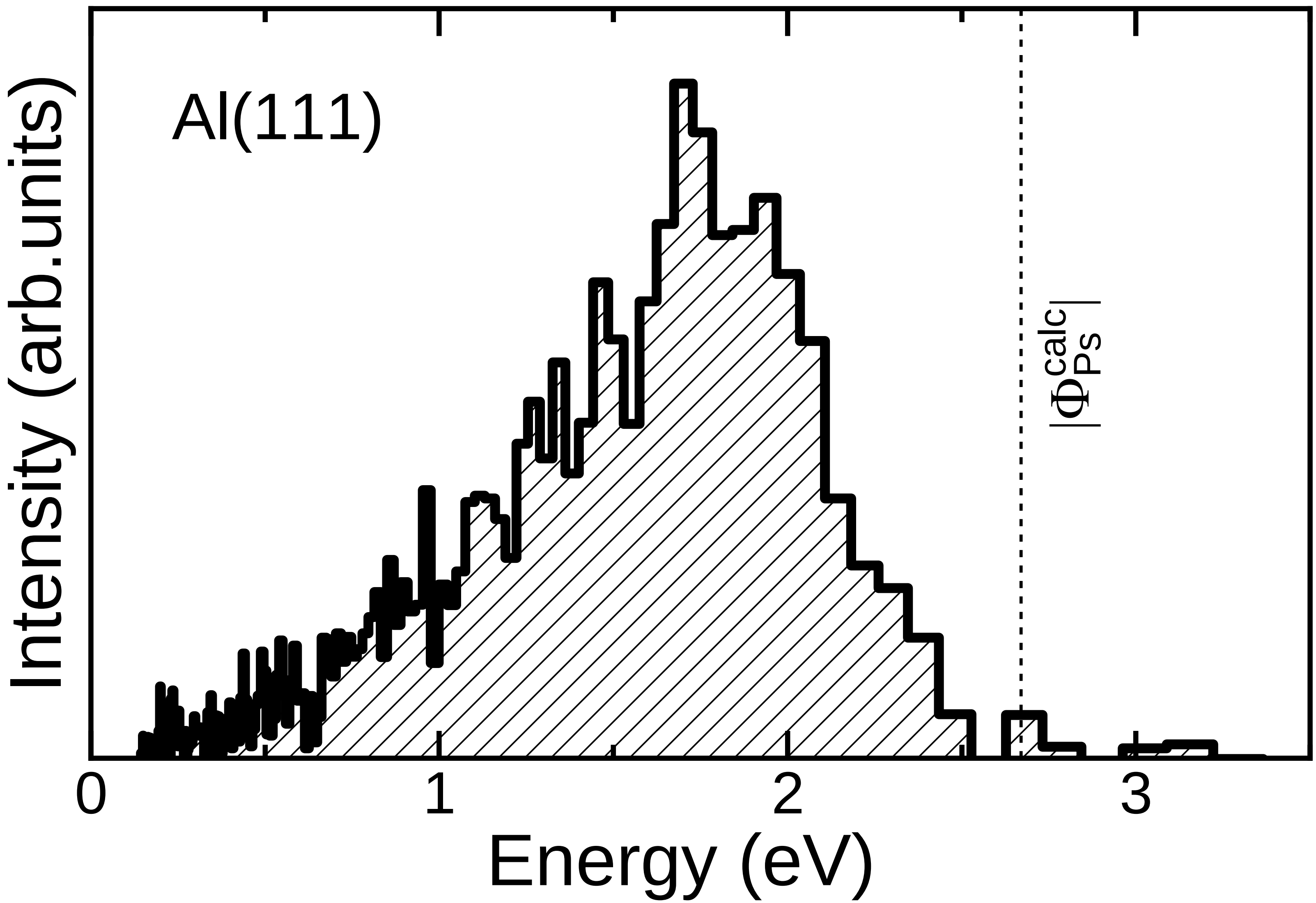
Transfer into UHV chamber
→ Heated to 1000 K
→ Cooling to 423 K, then measurement

Ps TOF spectra for Metals



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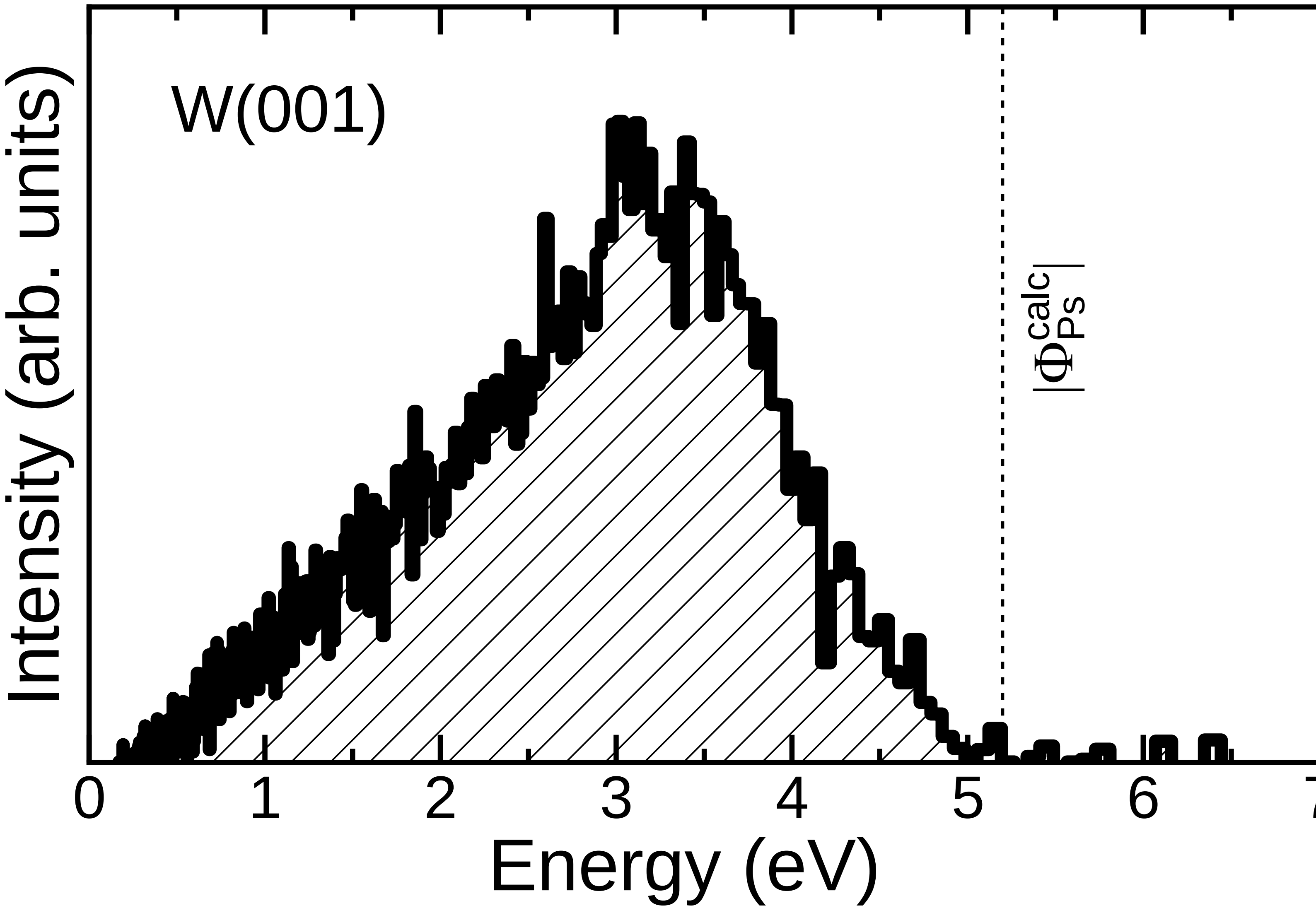
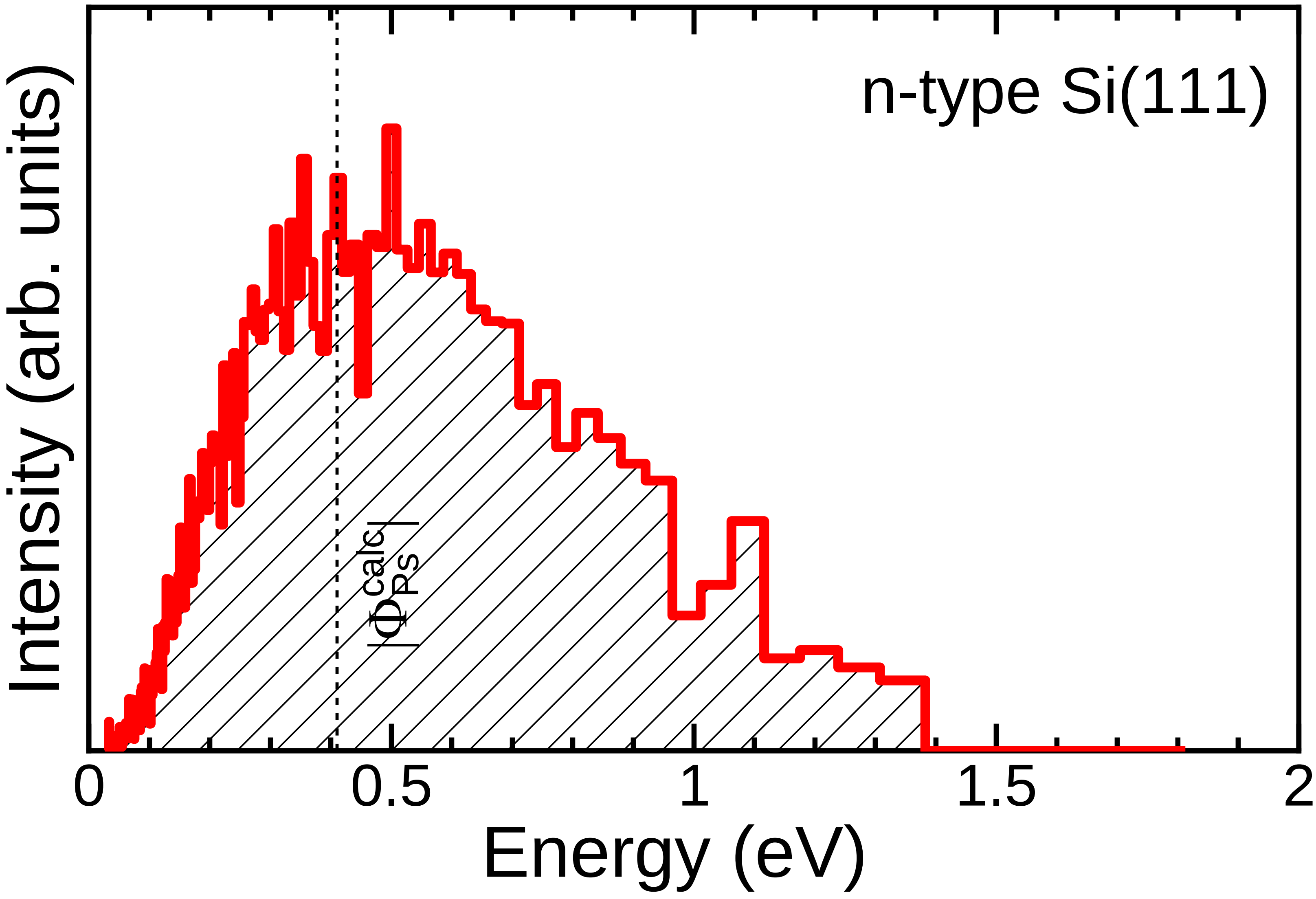


Ps TOF spectra for semiconductors



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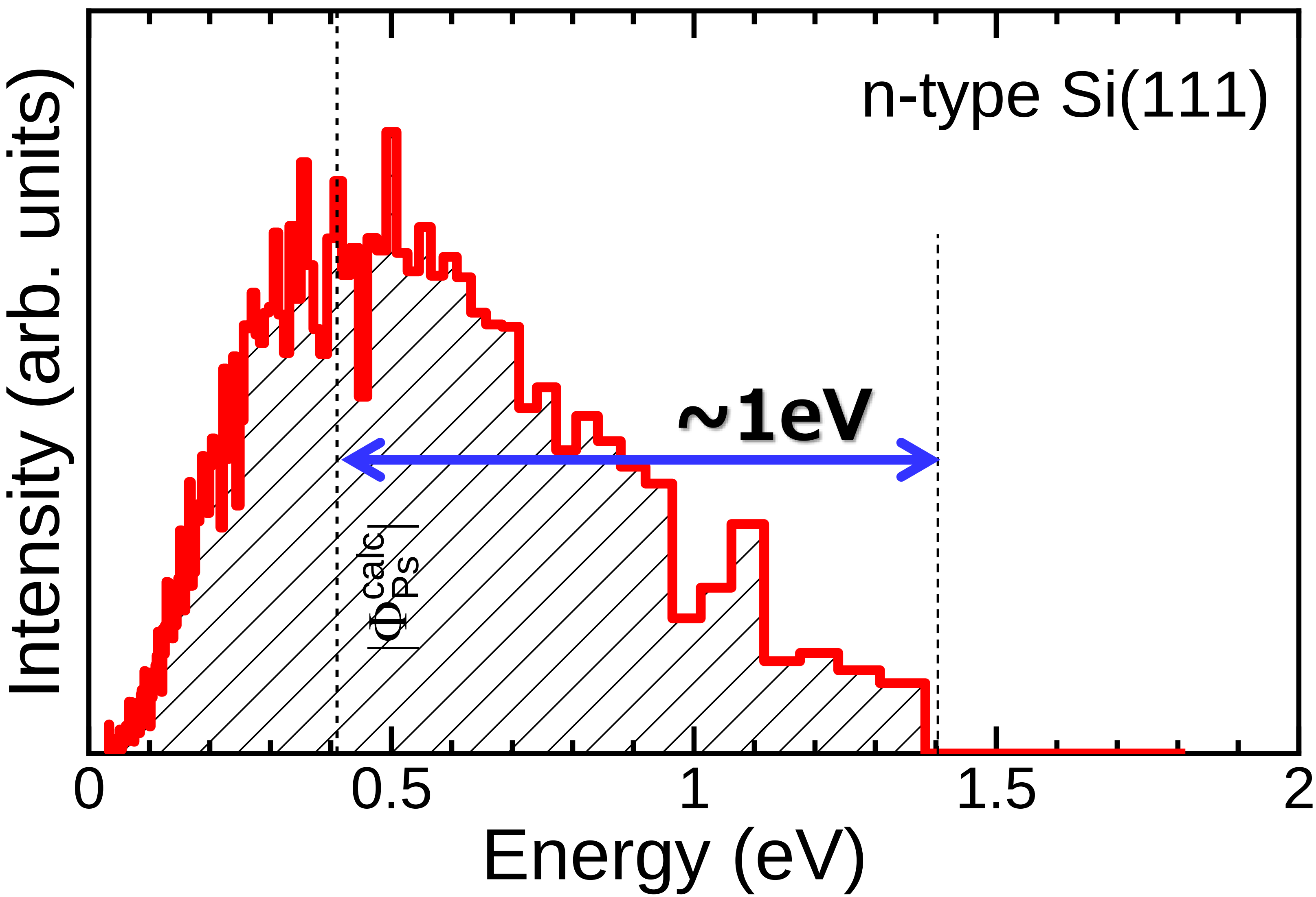

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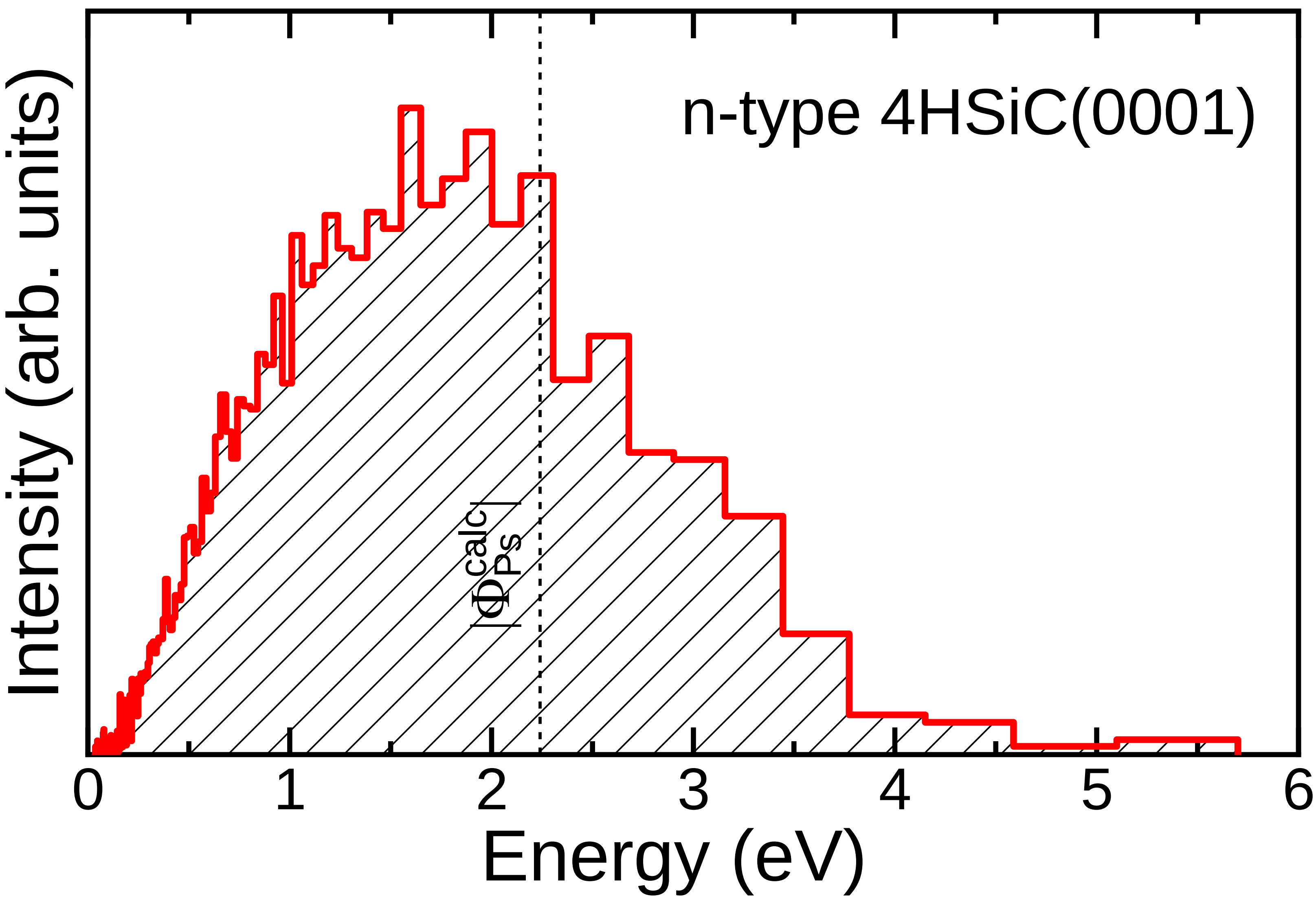

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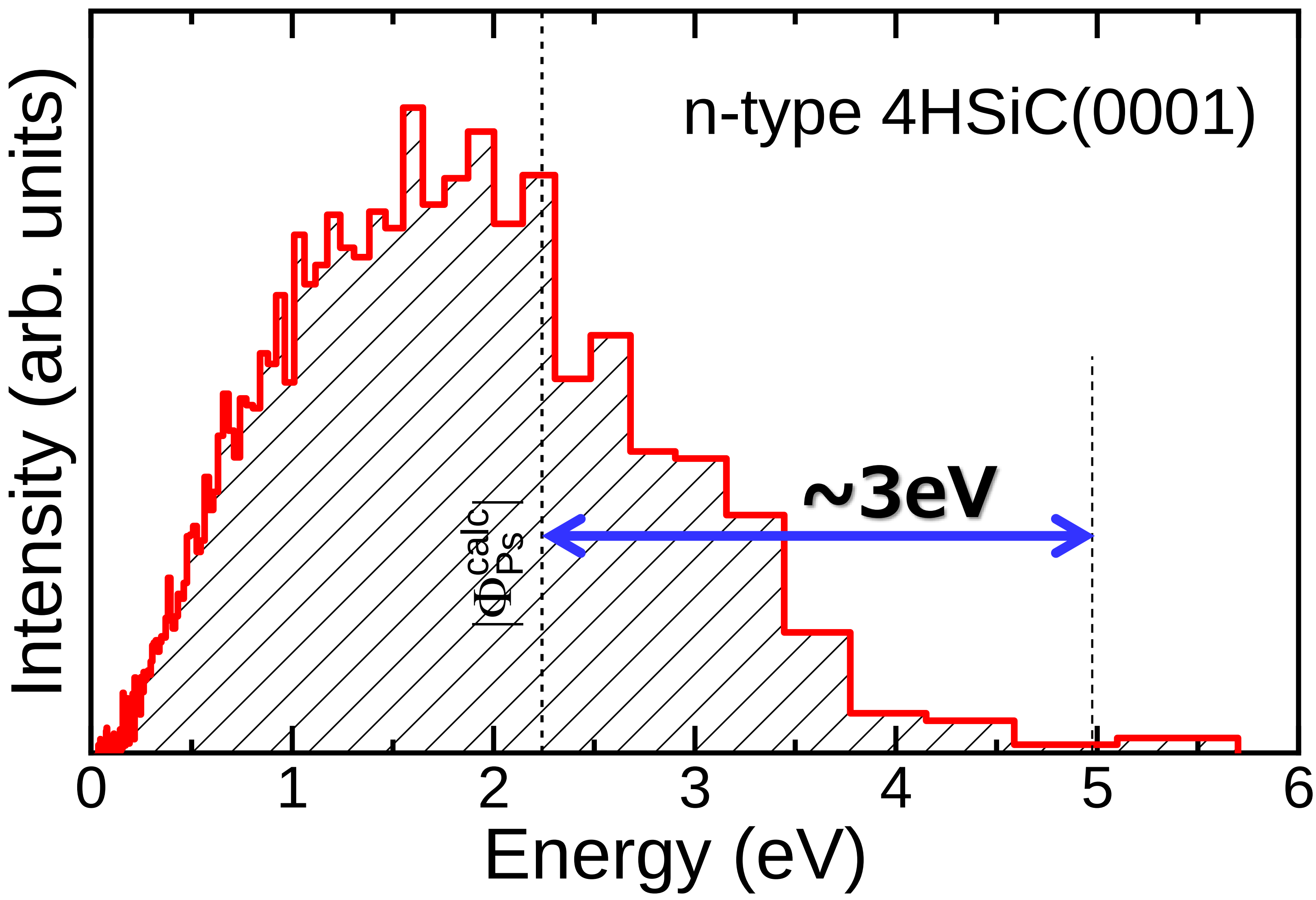

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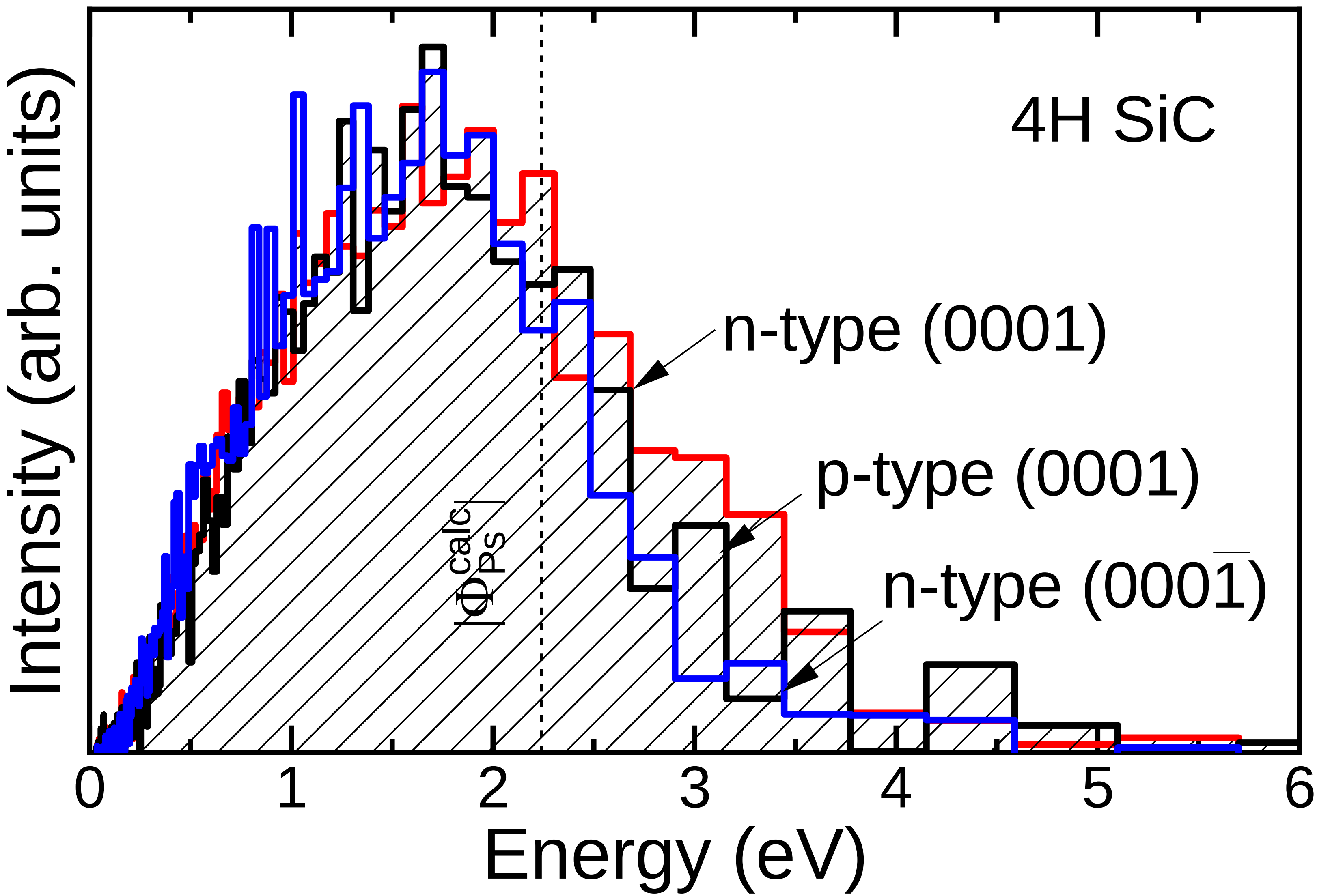

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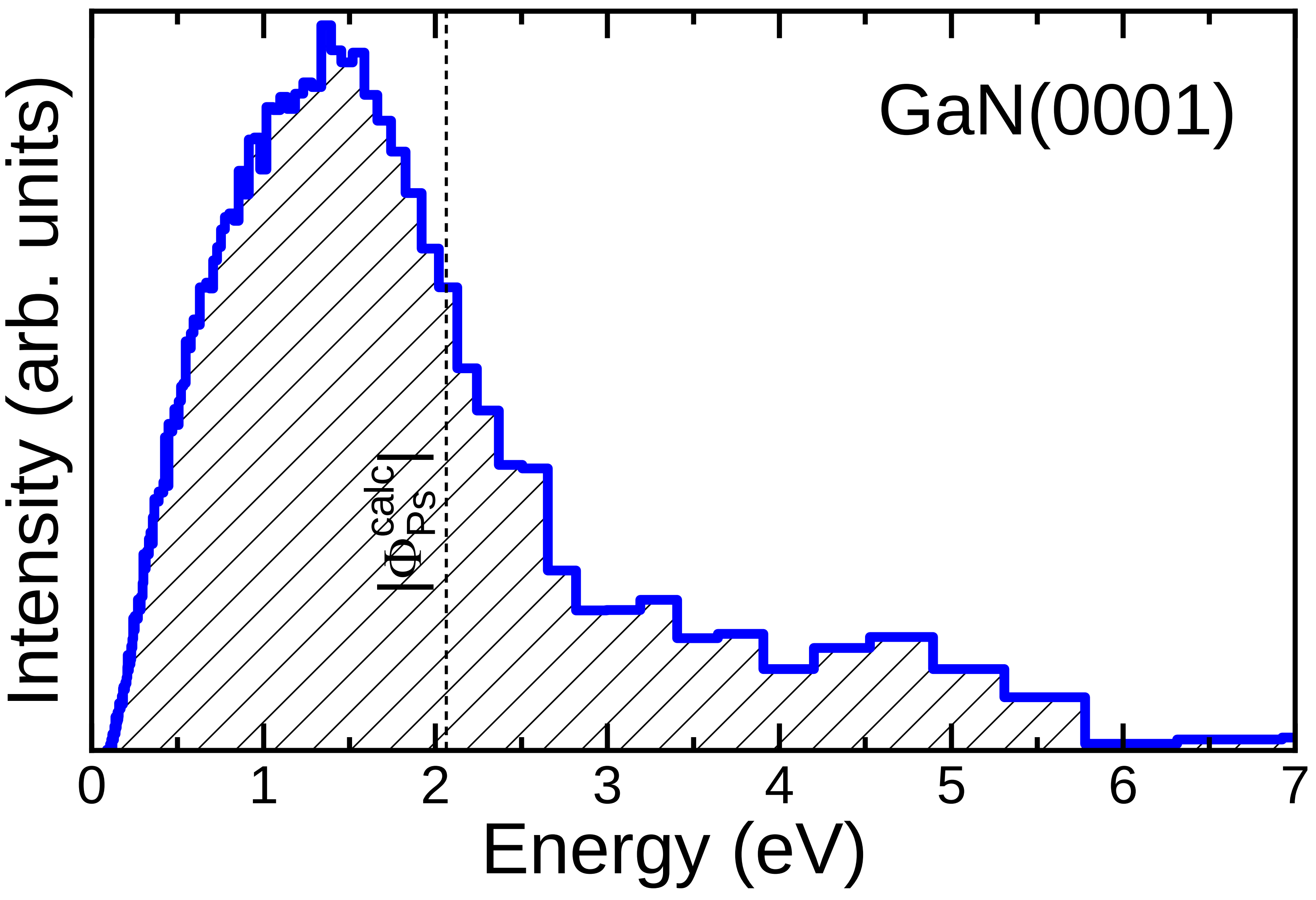

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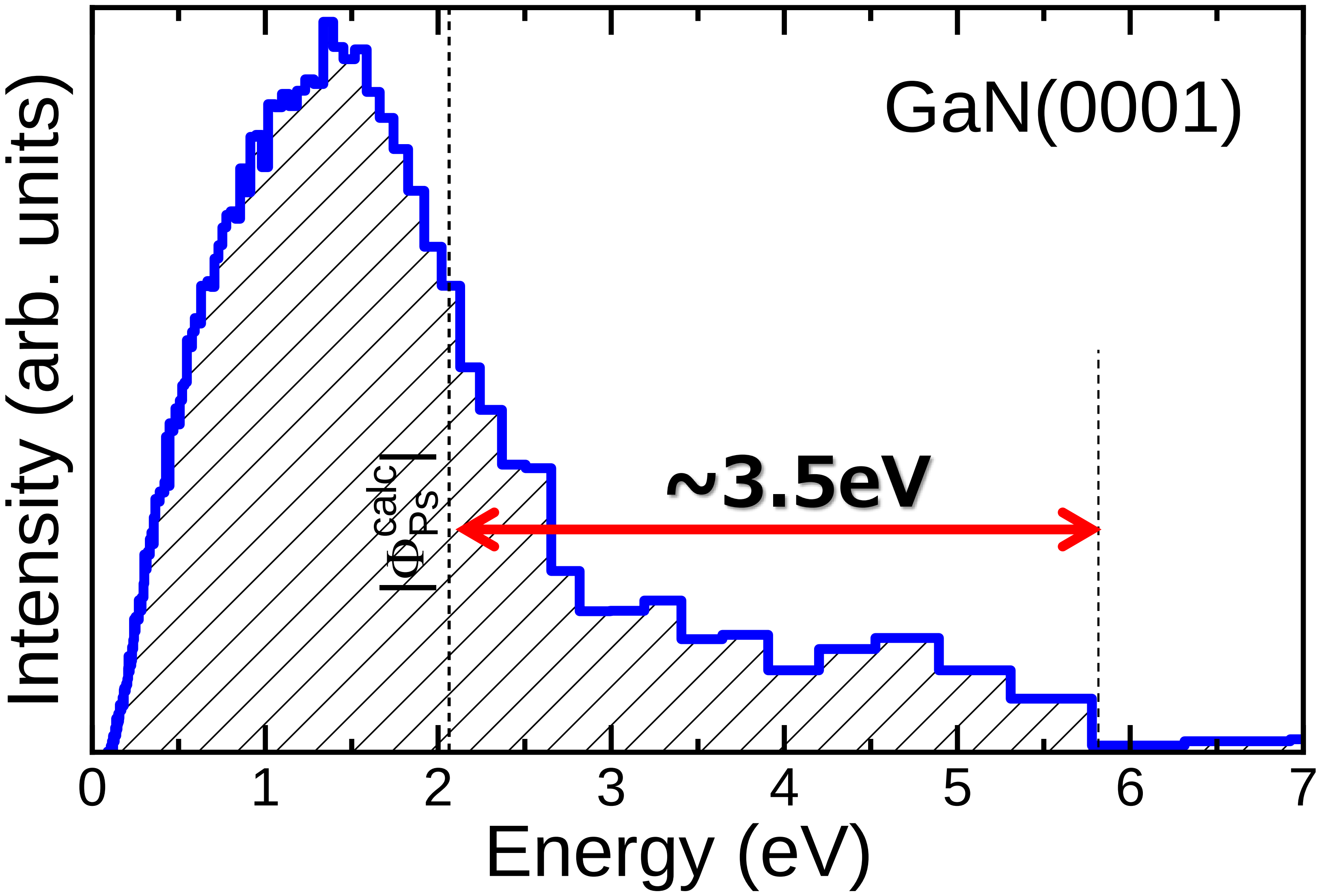

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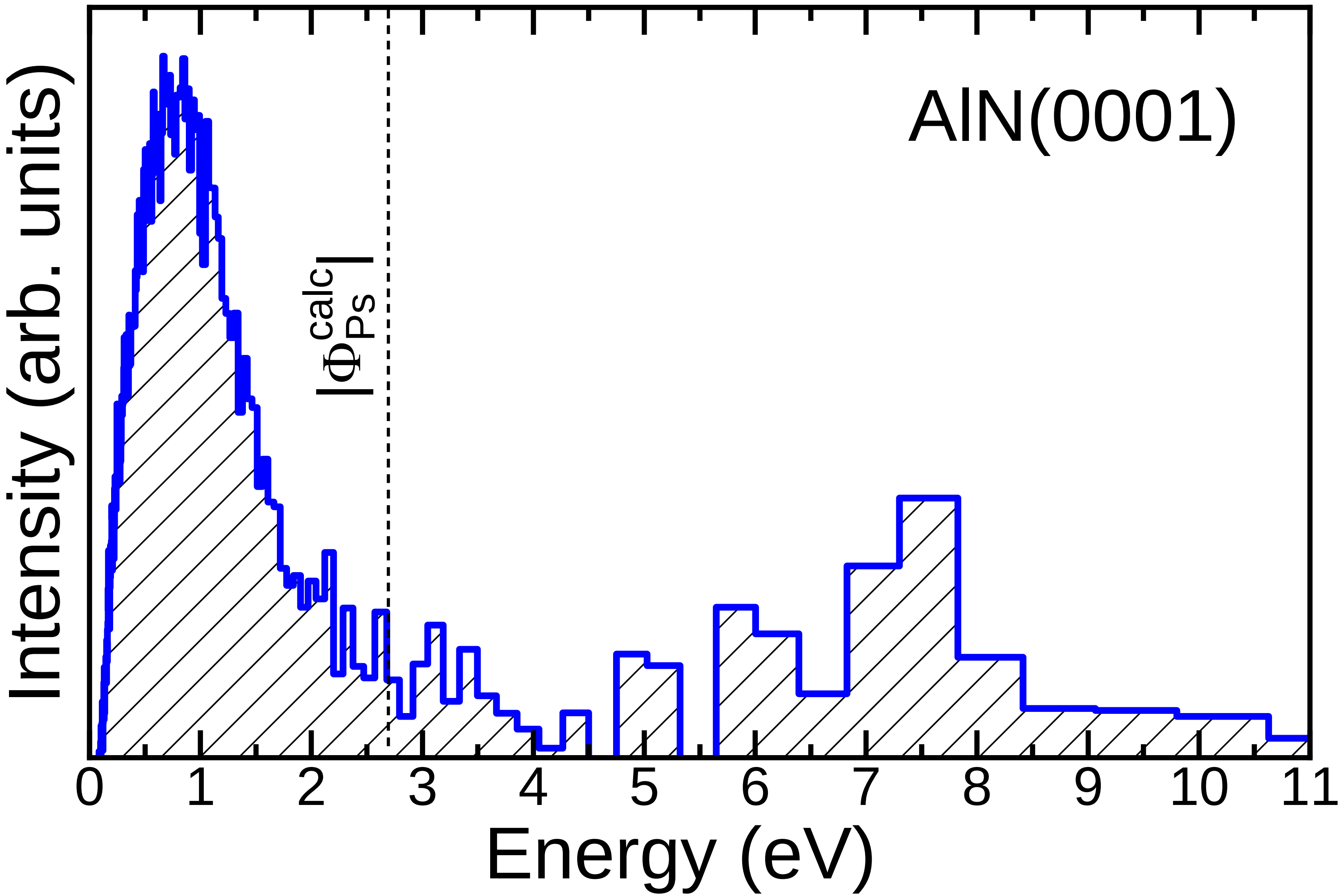

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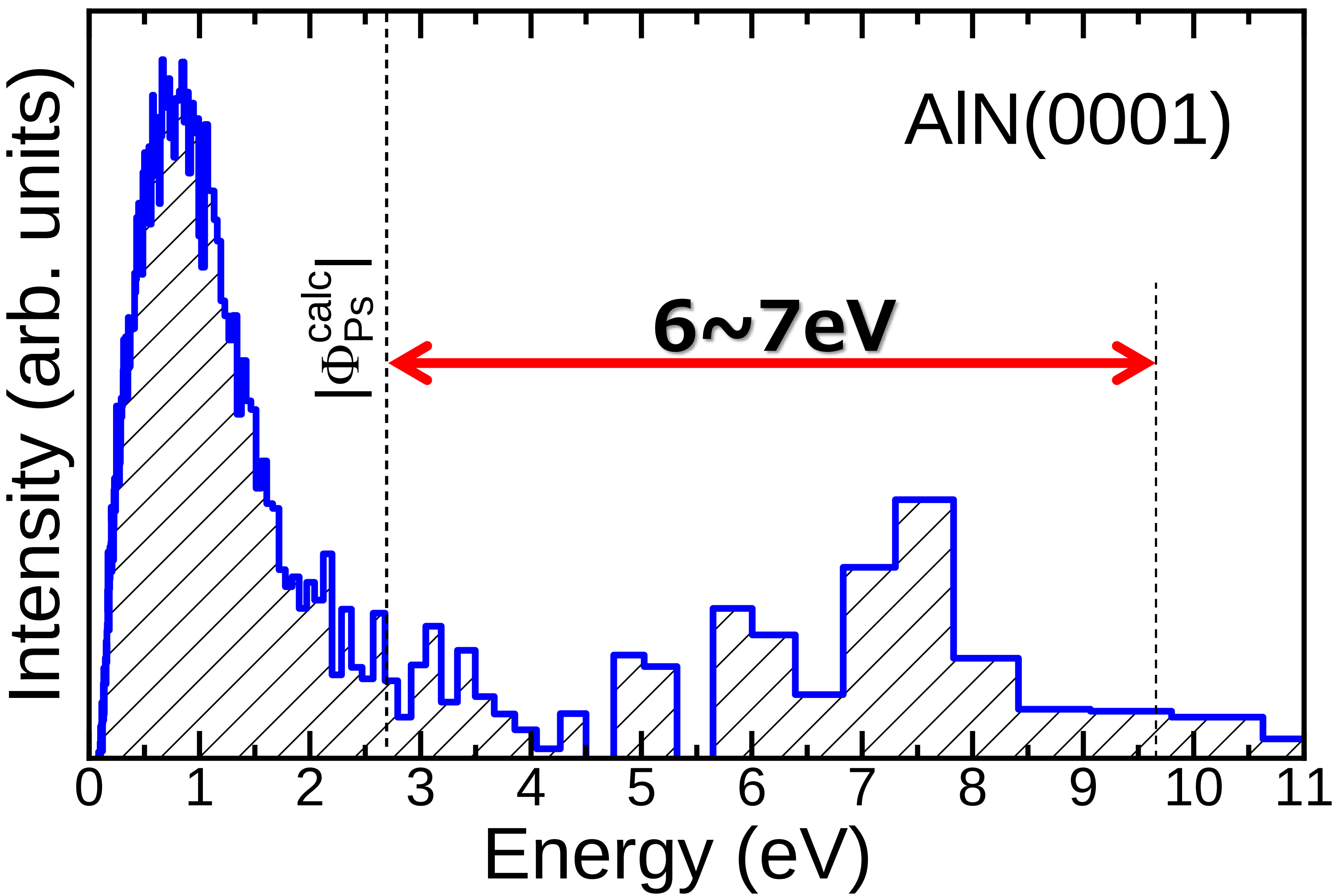
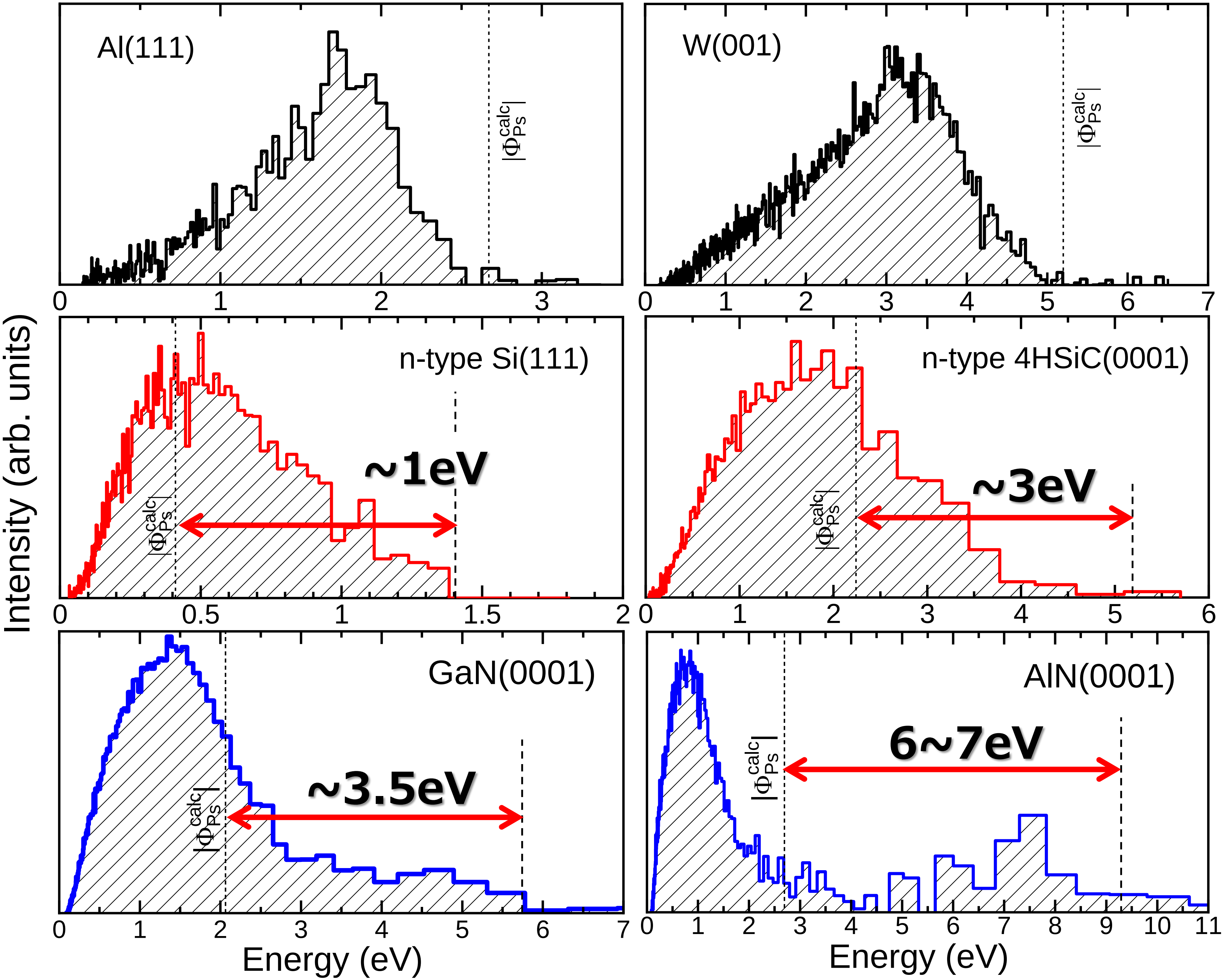
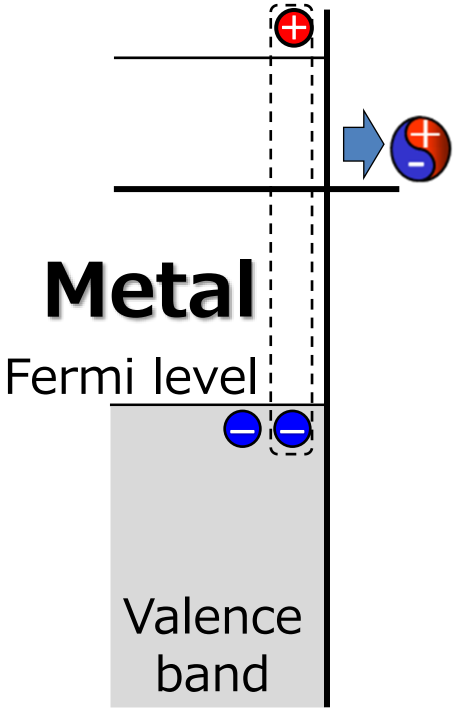
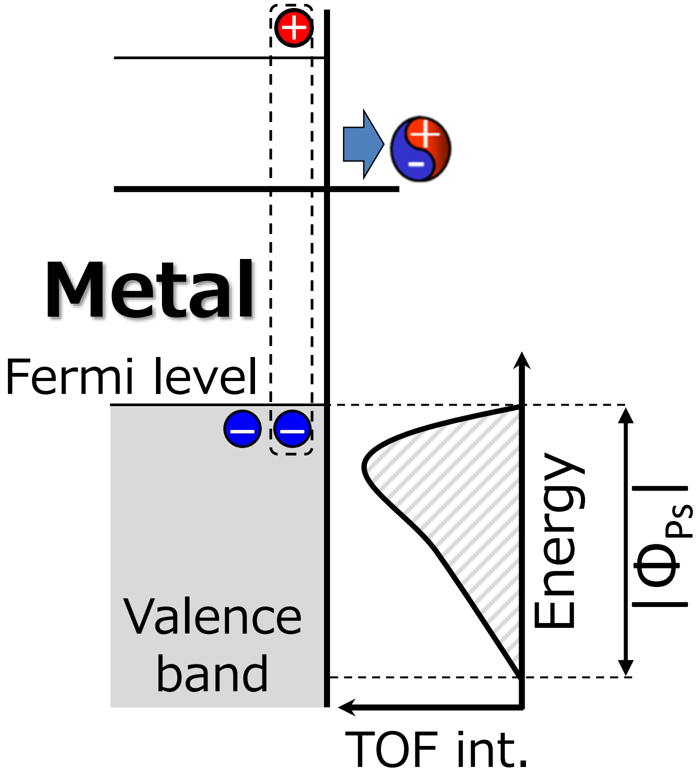




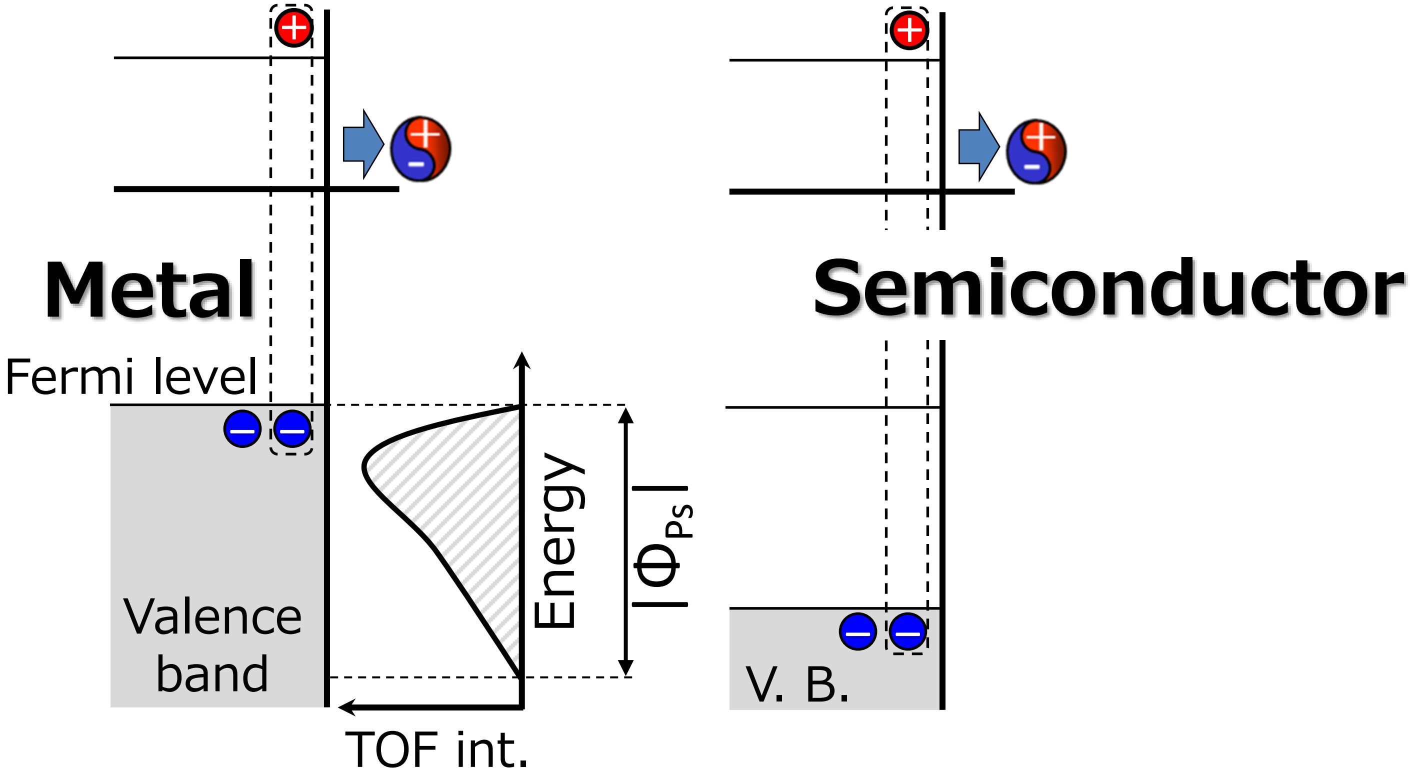
Al(111)
W(001)
n-type Si(111)
n-type 4HSiC(0001)
GaN(0001)
AlN(0001)
$|\Phi_{Ps}^{calc}|$
~1eV
~3eV
~3.5eV
6~7eV
Intensity (arb. units)
Energy (eV)
Energy (eV)



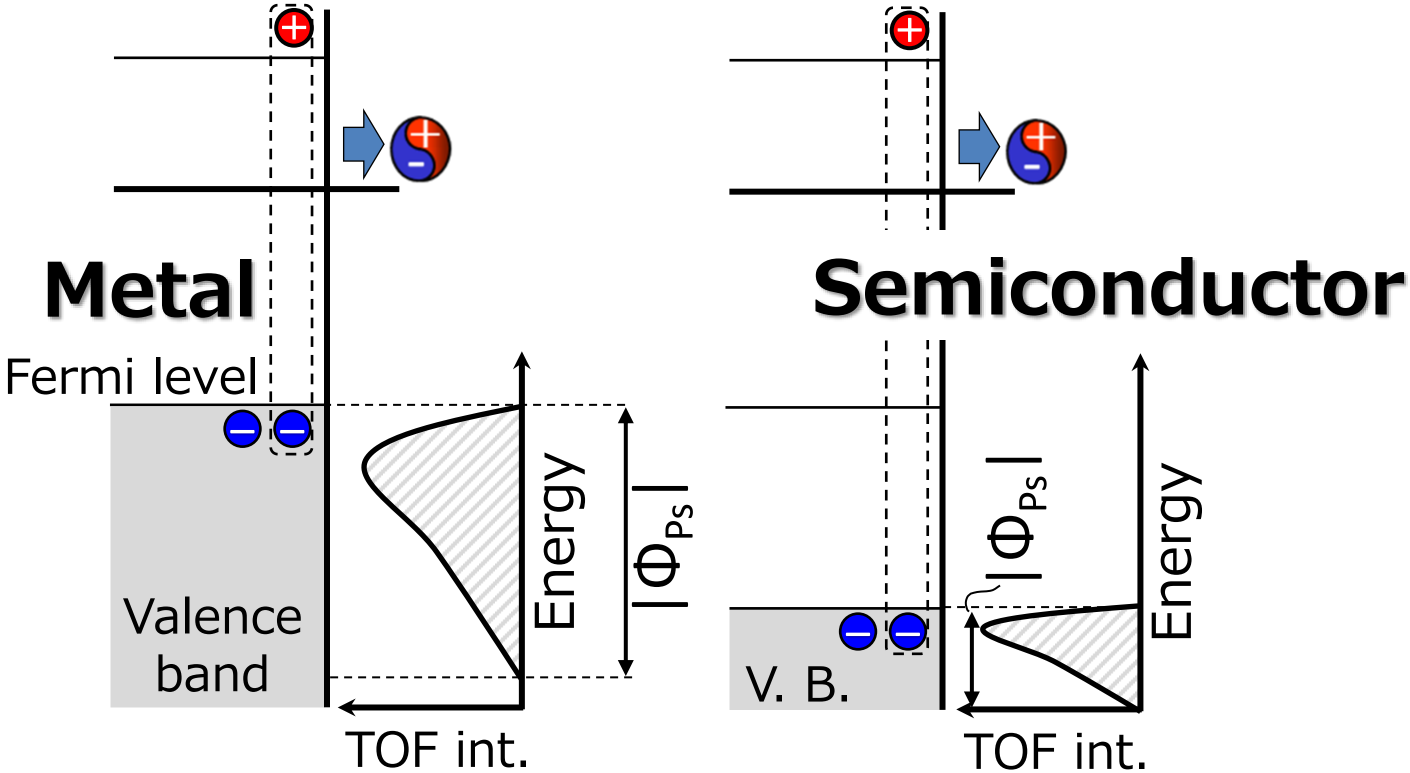
Metal
Fermi level
Valence
band



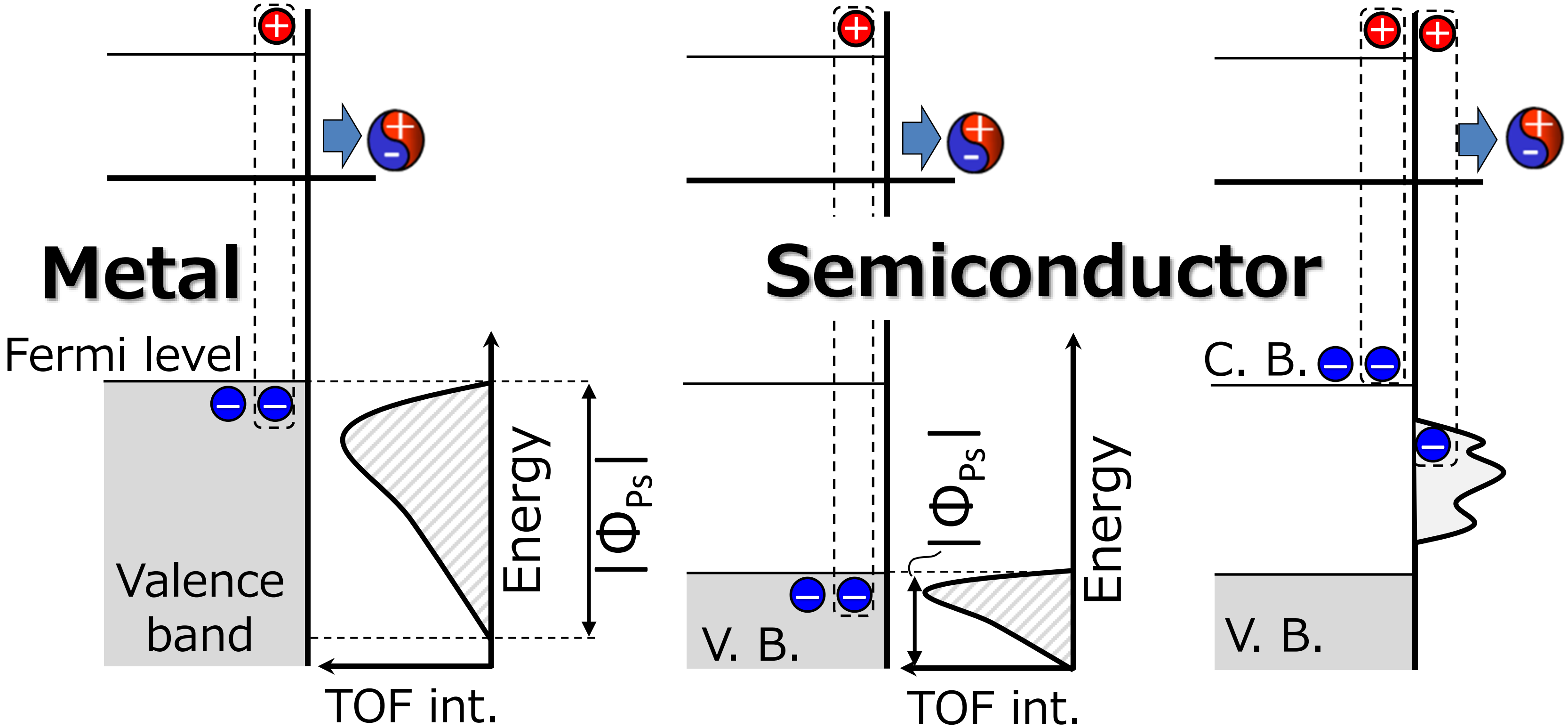
Metal
Fermi level
Valence band
Energy
$|\Phi_{Ps}|$
TOF int.

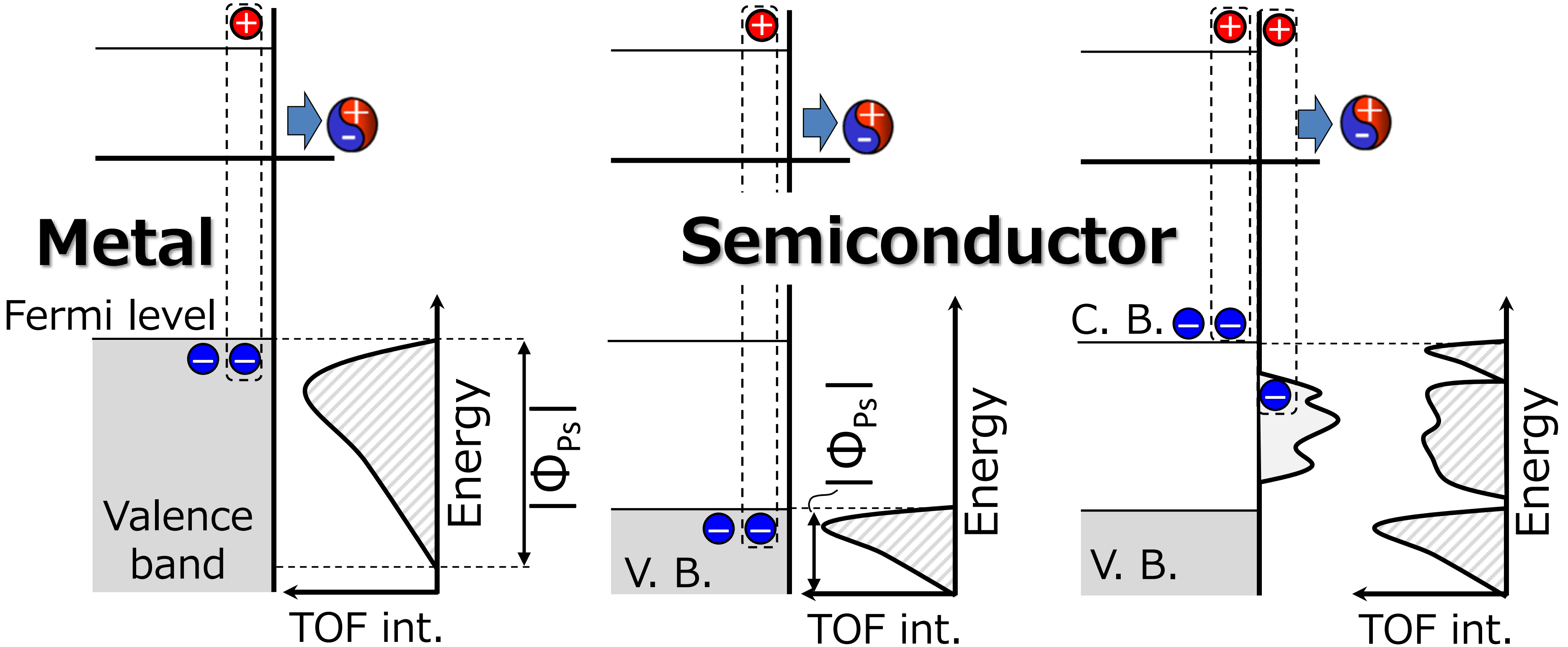


Metal
Fermi level
Valence band
Energy
|Φ_Ps|
TOF int.
Semiconductor
V. B.

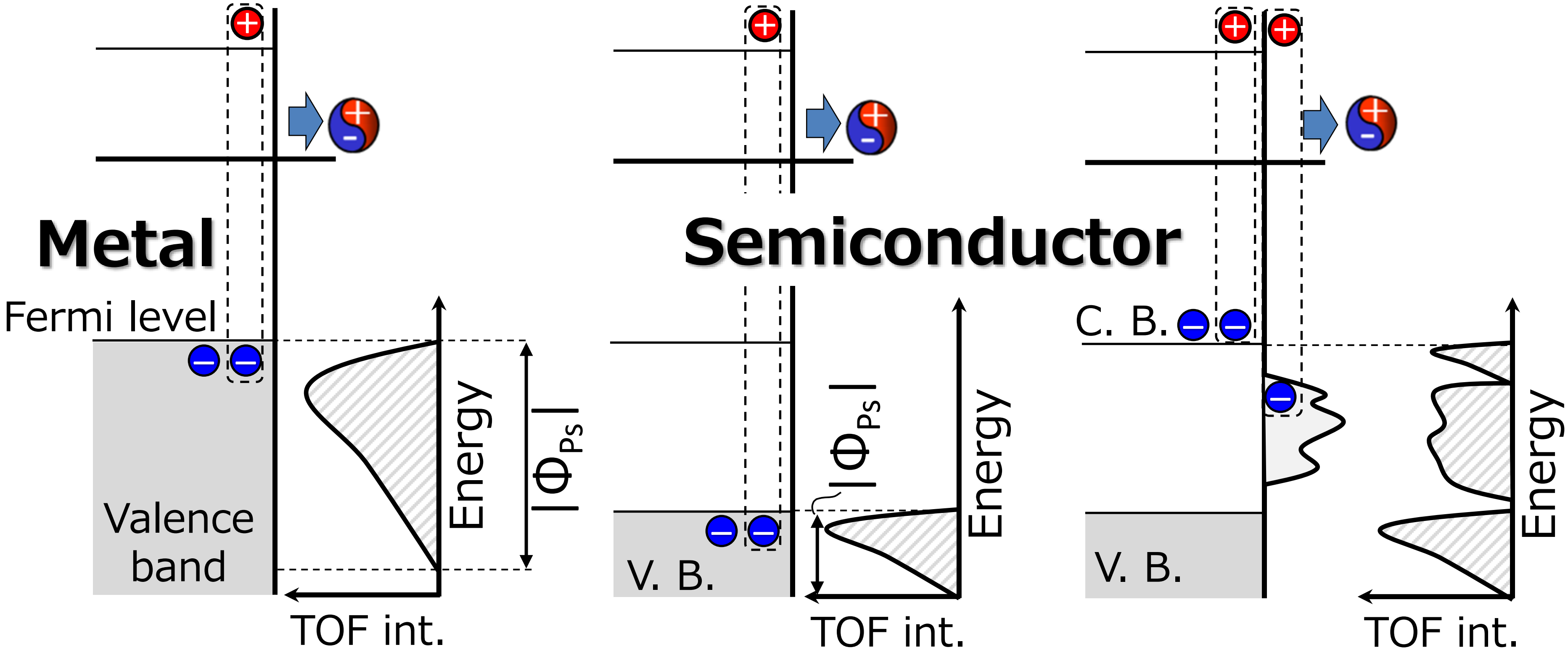


Metal
Fermi level
Valence band
Energy
$|\Phi_{Ps}|$
TOF int.
Semiconductor
V. B.
Energy
$|\Phi_{Ps}|$
TOF int.


Metal
Fermi level
Valence band
Energy
|Φ_Ps|
TOF int.
Semiconductor
V. B.
|Φ_Ps|
Energy
TOF int.
C. B.
V. B.

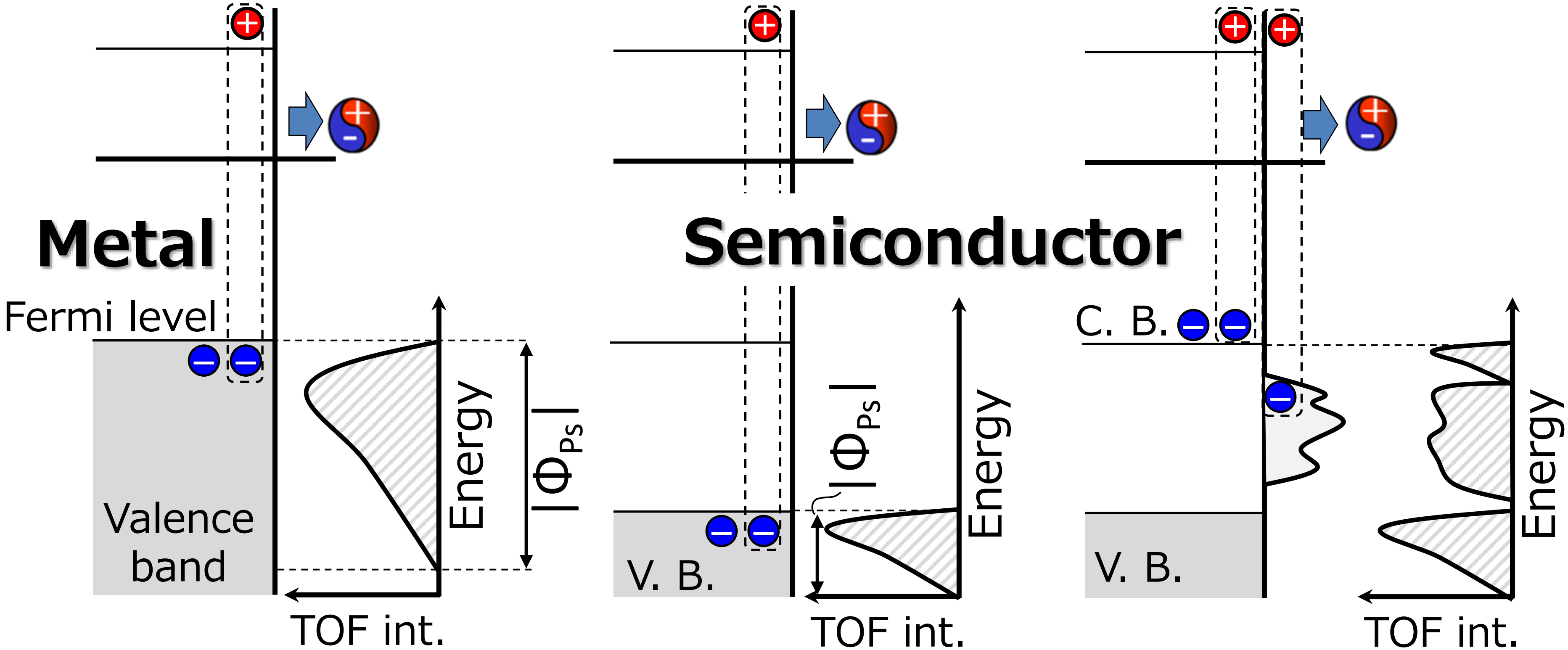


Metal
Fermi level
Valence band
Energy
|Φ_Ps|
TOF int.
Semiconductor
V. B.
|Φ_Ps|
Energy
TOF int.
C. B.
V. B.
Energy
TOF int.



Maximum Ps energy from $|\Phi_{Ps}|$

AlN: **6~7eV**
GaN: **~3.5eV**
SiC: **~3eV**
Si: **~1eV**



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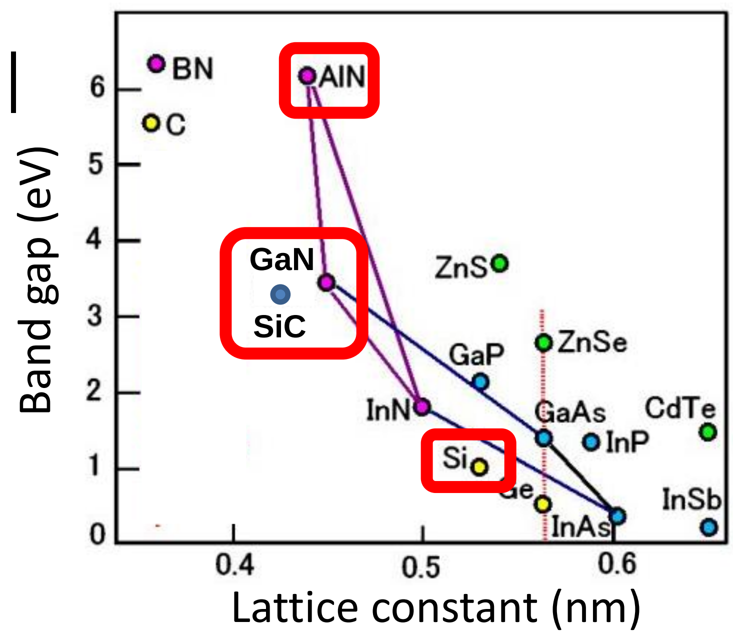

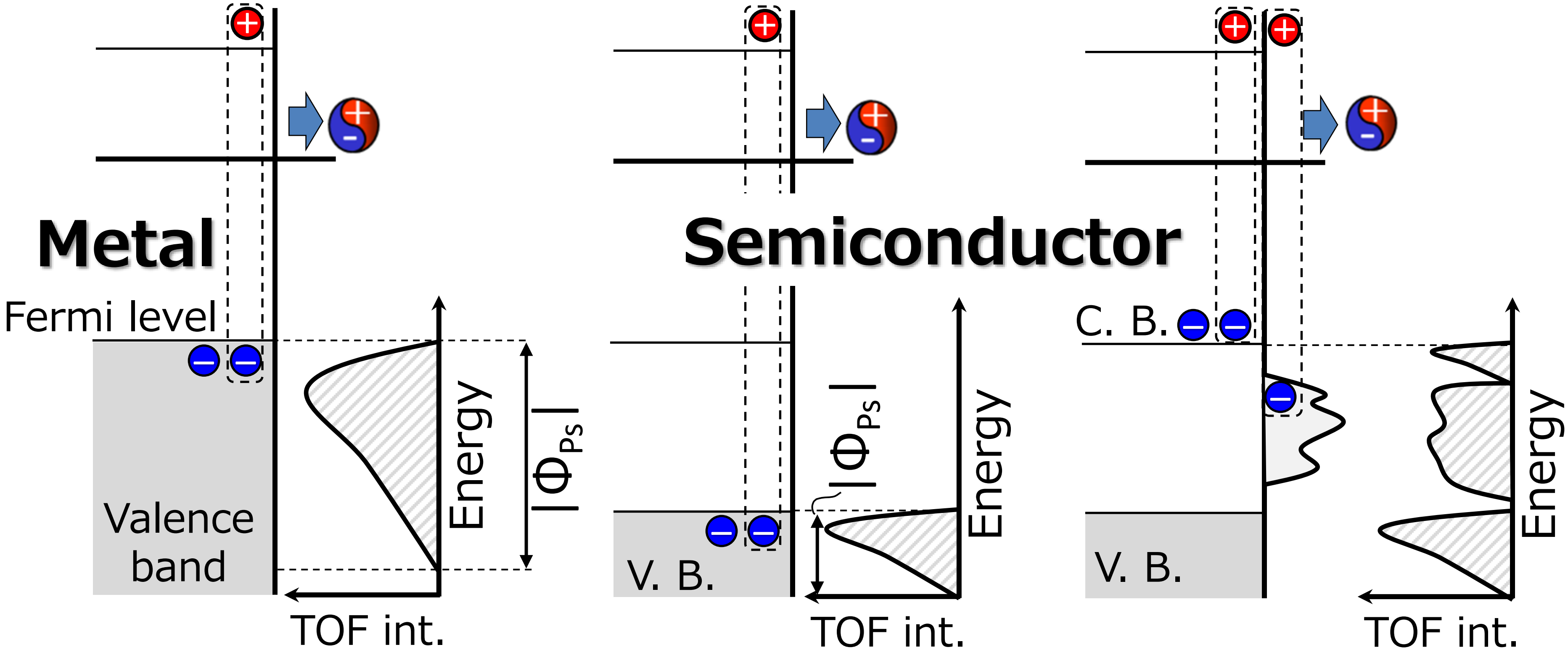

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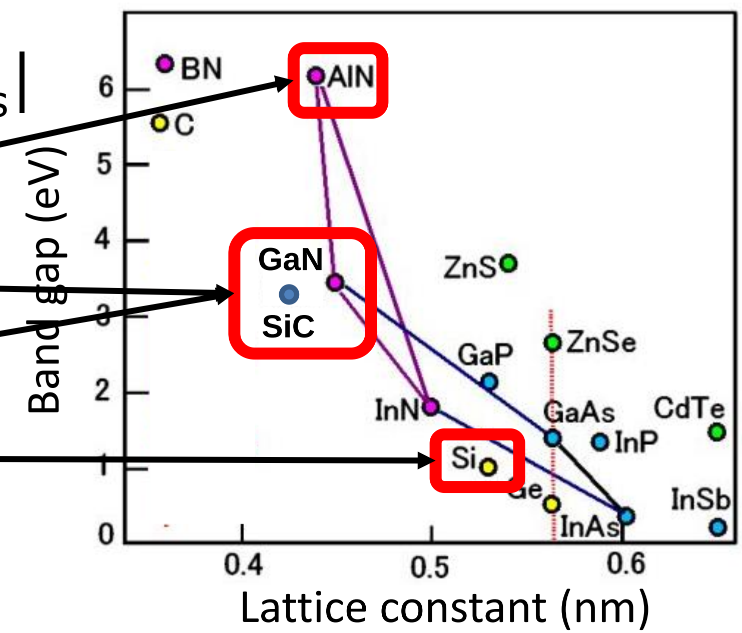
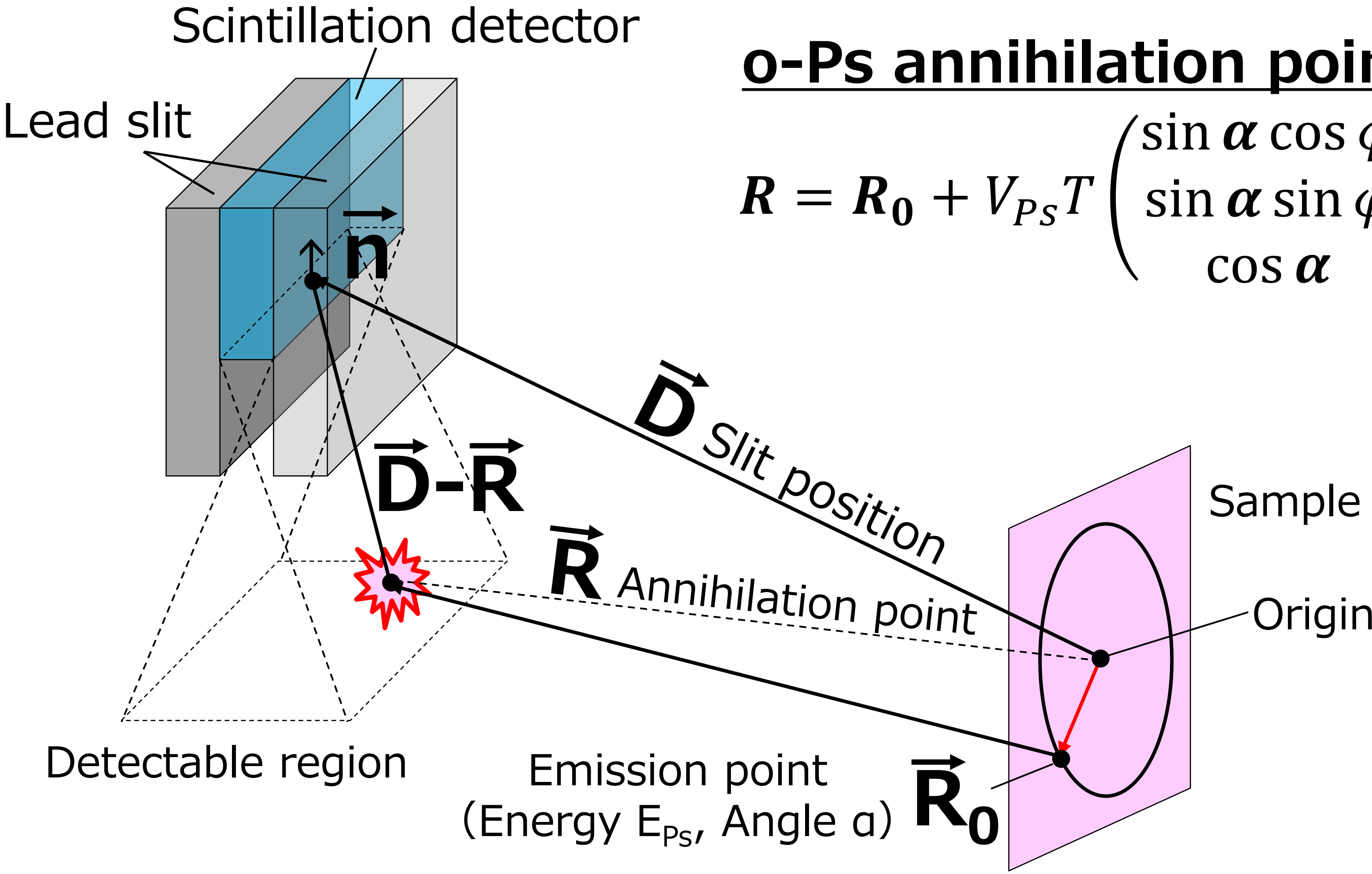


Ps TOF Monte Carlo Simulation (by Maekawa)



o-Ps annihilation point

$$\boldsymbol{R} = \boldsymbol{R_0} + V_{Ps}T\begin{pmatrix}\sin\boldsymbol{\alpha}\cos\varphi \\ \sin\boldsymbol{\alpha}\sin\varphi \\ \cos\boldsymbol{\alpha}\end{pmatrix}$$

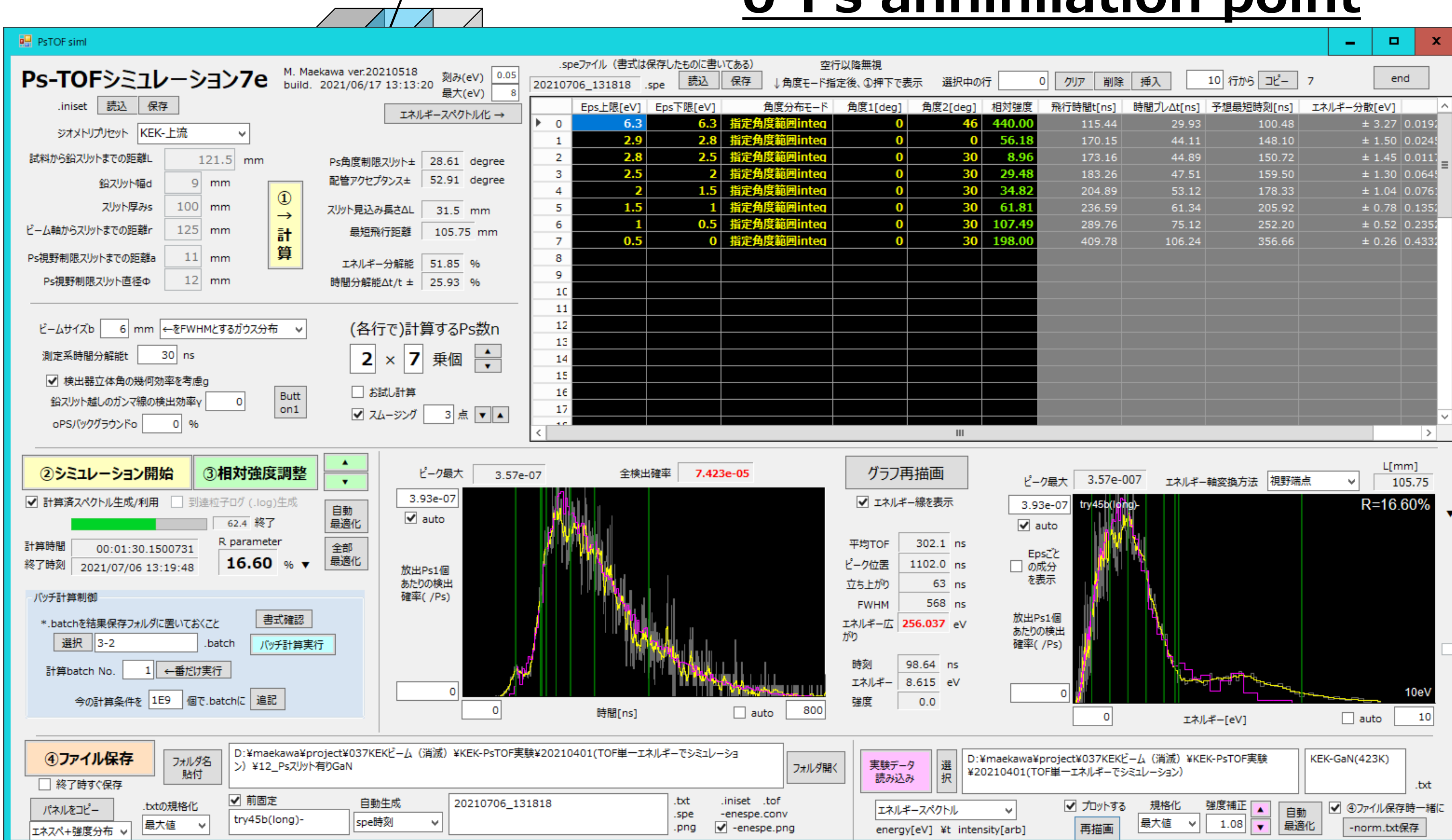
Ps TOF spectrum

$$\boldsymbol{N}_{Ps}(T) \propto \left[\iint_S \frac{ds((\boldsymbol{D}-\boldsymbol{R})\cdot\boldsymbol{n})}{(D-R)^3} ds\, exp\left(\frac{-T}{142[ns]}\right)\right] \otimes G(t)$$

Ps TOF Monte Carlo Simulation (by Maekawa)

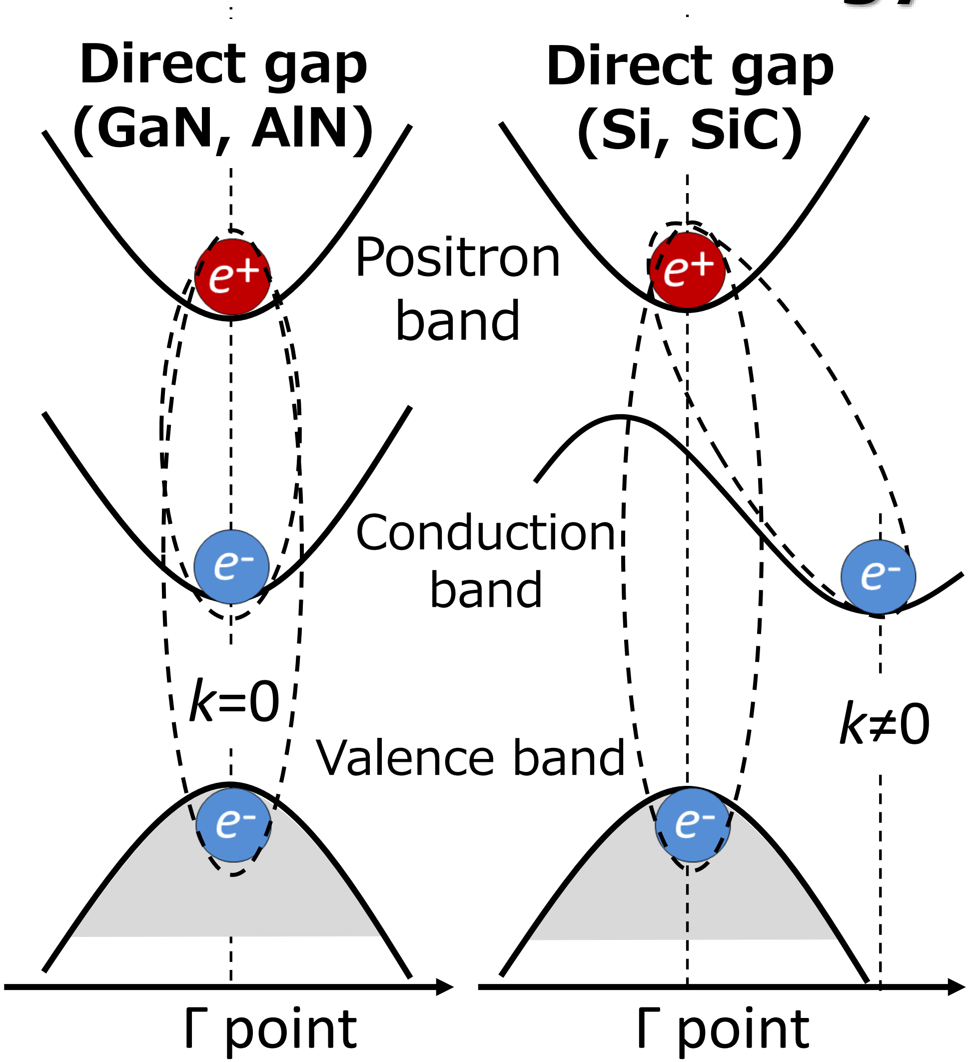
Scintillation detector

o-Ps annihilation point



Ps TOF spectrum $N_{Ps}(t)$ ... $\left[\iint_s \right.$ ... $(D-R)^3$ ... $\left. \left(142[ns]\right)\right]$ ... (t)

How to think Ps energy and angle?



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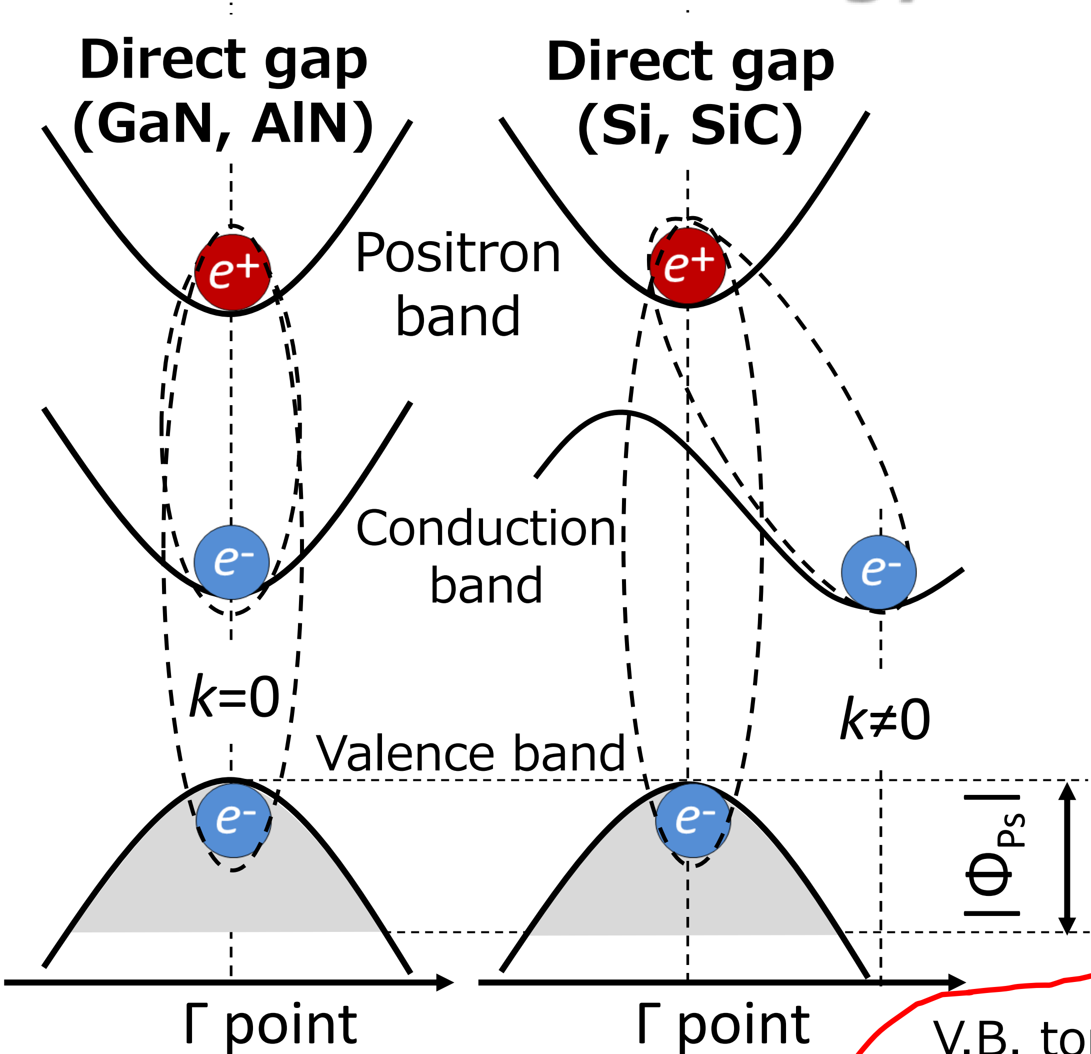
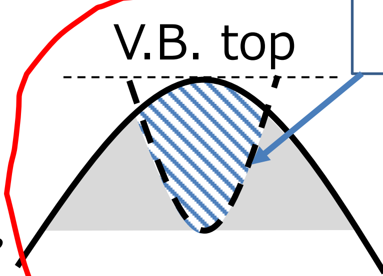


Valence



Ps energy distribution

$$0 \leq E_{Ps} \leq -\Phi_{Ps}$$

Ps angle distribution

Pickable wave number in band dispersion

$$0 \leq k_{//} \leq \sqrt{-4m\Phi_{Ps} / \hbar^2}$$

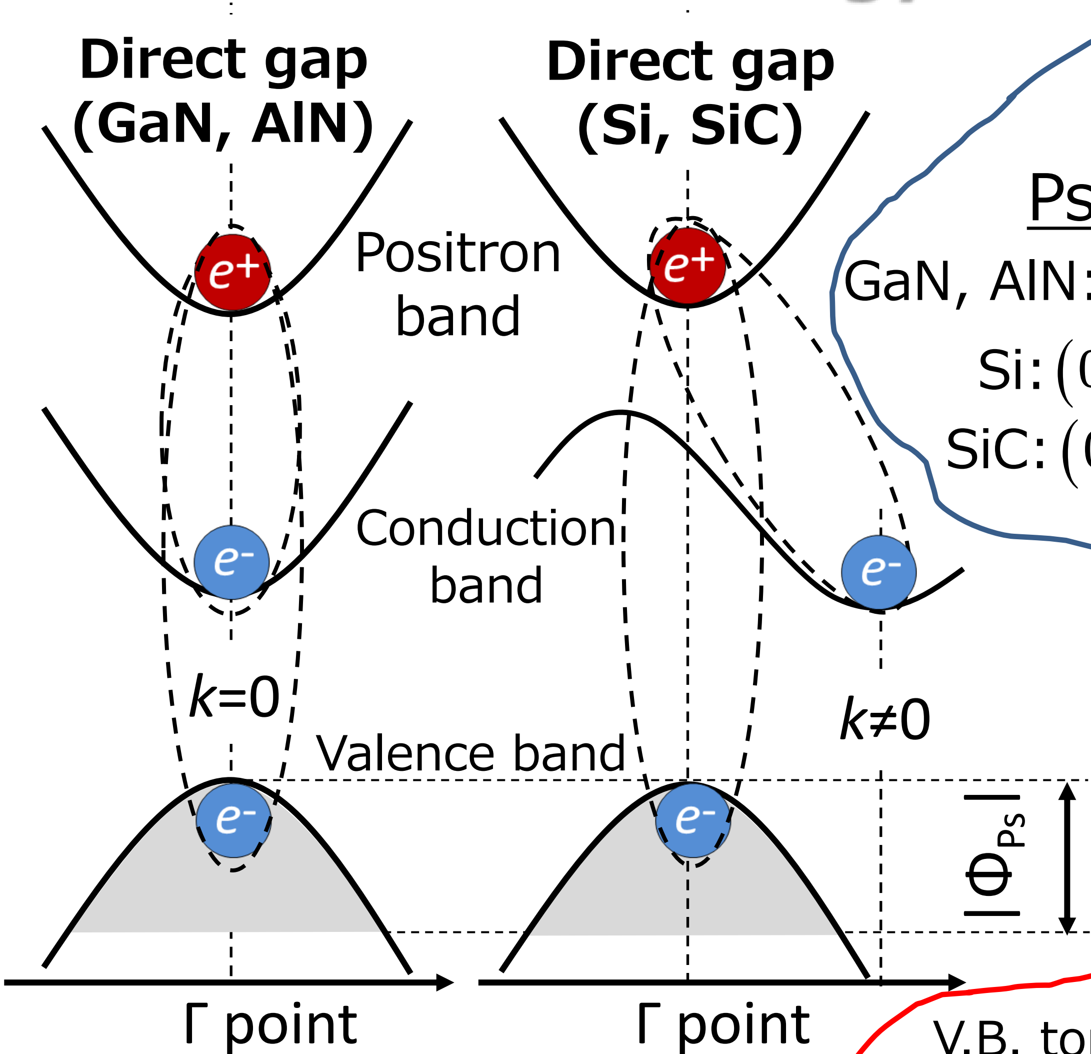
Ex. Φ_{Ps}=3eV roughly

$$-20^\circ \leq \theta_{Ps} \leq 20^\circ$$

+ Phonon broadening

How to think Ps energy and angle?

Conduct.



Ps energy

$$E_{Ps} = -\Phi_{Ps} + E_G$$

Ps angle distribution

GaN, AlN: $\theta_{Ps} = 0^\circ$ **+Phonon broadening**

Si: $(0.85,0,0)2\pi/a$ $\theta_{Ps} = 45^\circ$

SiC: $(0.5,0,0)4\pi/(\sqrt{3}a)$ $\theta_{Ps} = 51^\circ$

+Phonon broadening

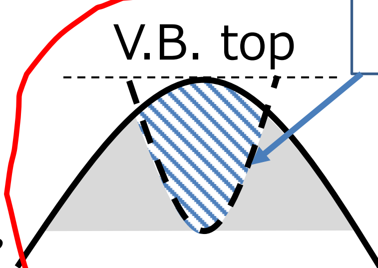
Ps energy distribution

$$0 \le E_{Ps} \le -\Phi_{Ps}$$

Ps angle distribution

Pickable wave number in band dispersion

$$0 \le k_{//} \le \sqrt{-4m\Phi_{Ps}/\hbar^2}$$



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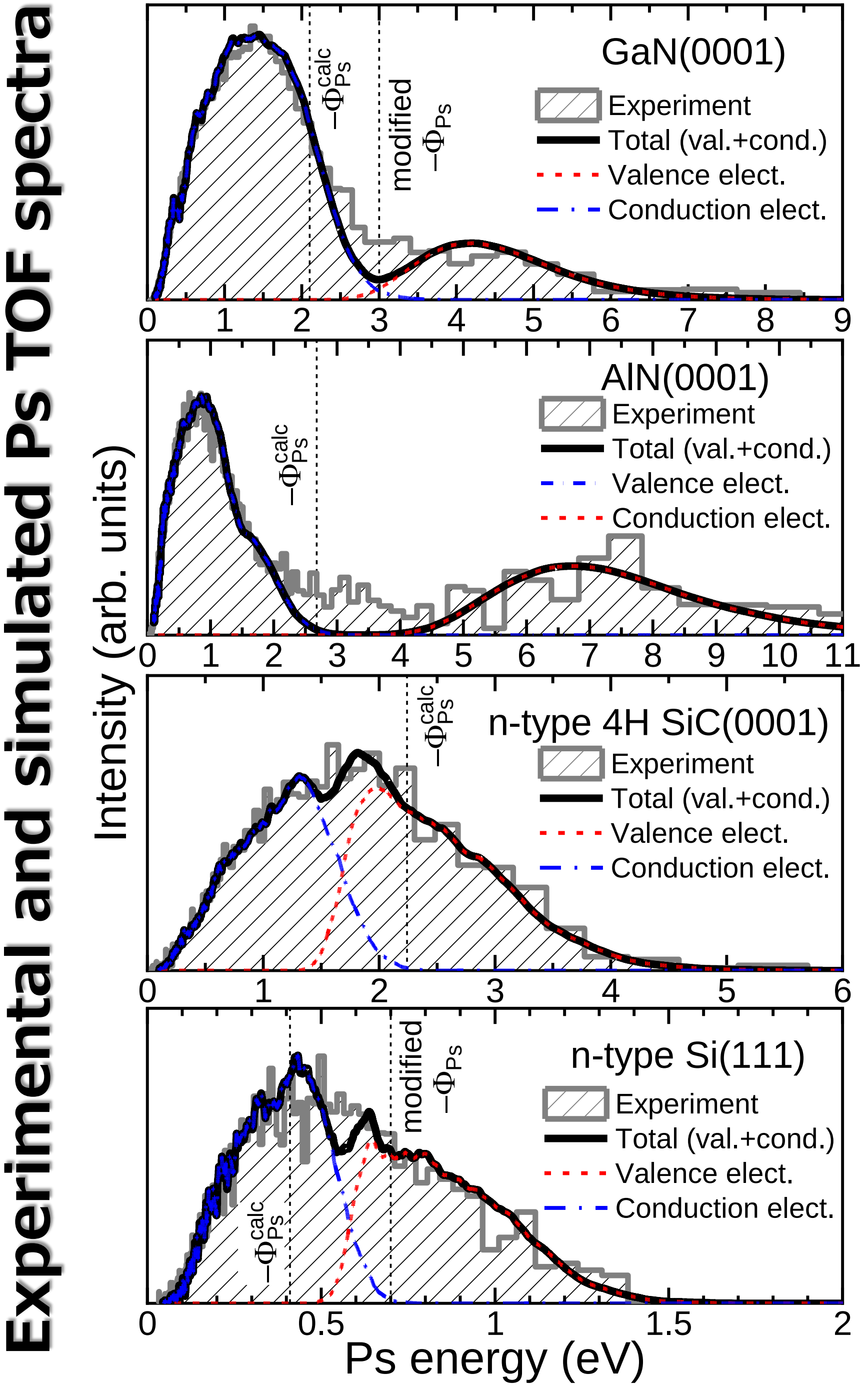
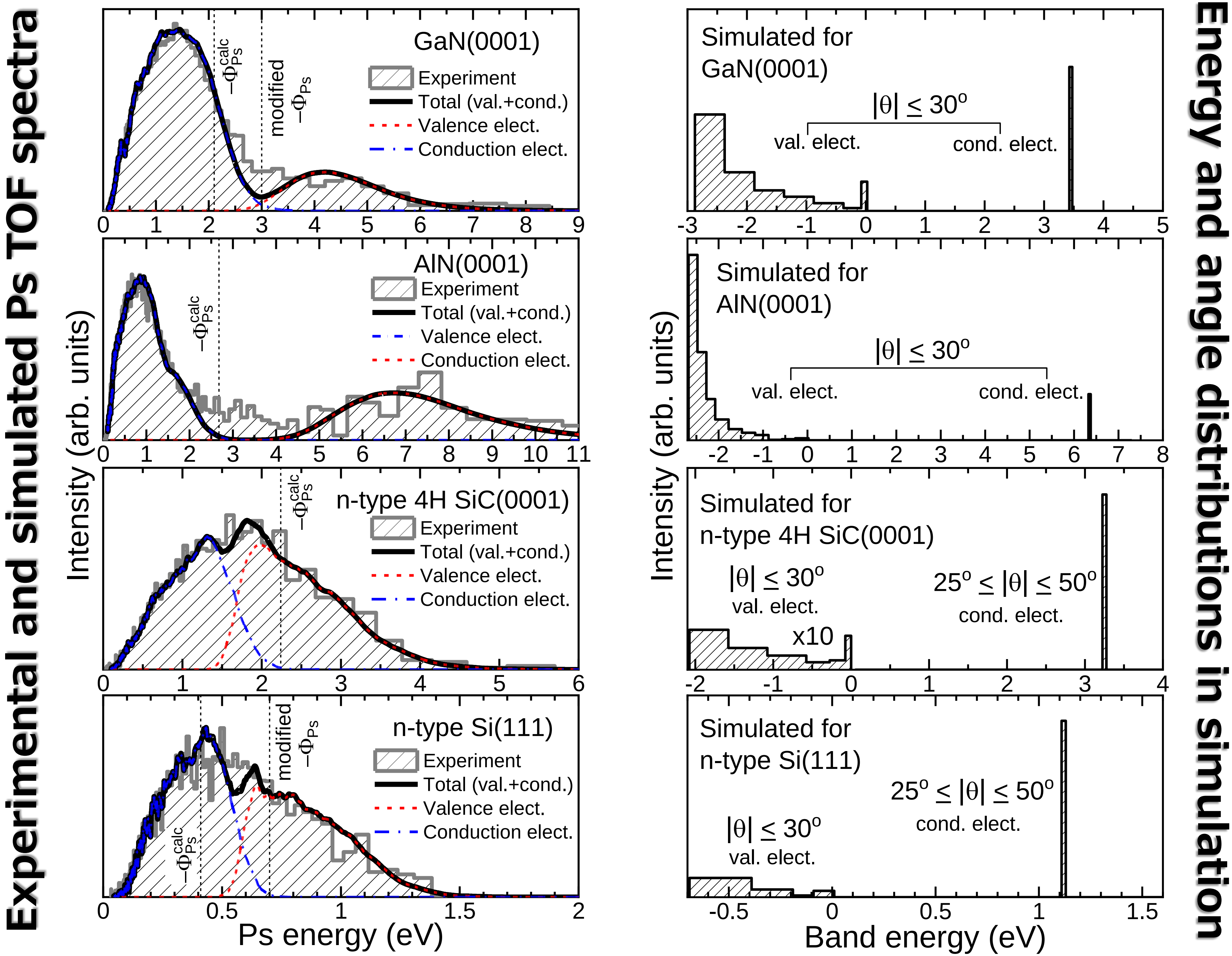


Experimental and simulated Ps TOF spectra
Intensity (arb. units)
Ps energy (eV)
GaN(0001)
$-\Phi_{Ps}^{calc}$
modified $-\Phi_{Ps}$
Experiment
Total (val.+cond.)
Valence elect.
Conduction elect.
AlN(0001)
$-\Phi_{Ps}^{calc}$
Experiment
Total (val.+cond.)
Valence elect.
Conduction elect.
n-type 4H SiC(0001)
$-\Phi_{Ps}^{calc}$
Experiment
Total (val.+cond.)
Valence elect.
Conduction elect.
n-type Si(111)
$-\Phi_{Ps}^{calc}$
modified $-\Phi_{Ps}$
Experiment
Total (val.+cond.)
Valence elect.
Conduction elect.



Experimental and simulated Ps TOF spectra
Energy and angle distributions in simulation
GaN(0001)
Experiment
Total (val.+cond.)
Valence elect.
Conduction elect.
$-\Phi_{Ps}^{calc}$
modified $-\Phi_{Ps}$
AlN(0001)
n-type 4H SiC(0001)
n-type Si(111)
Intensity (arb. units)
Ps energy (eV)
Simulated for GaN(0001)
$|\theta| \leq 30^o$
val. elect.
cond. elect.
Simulated for AlN(0001)
Simulated for n-type 4H SiC(0001)
$25^o \leq |\theta| \leq 50^o$
x10
Simulated for n-type Si(111)
Band energy (eV)

Summary and prospects

Ps emission from Si, SiC, GaN and AlN has been studied through Ps TOF method.

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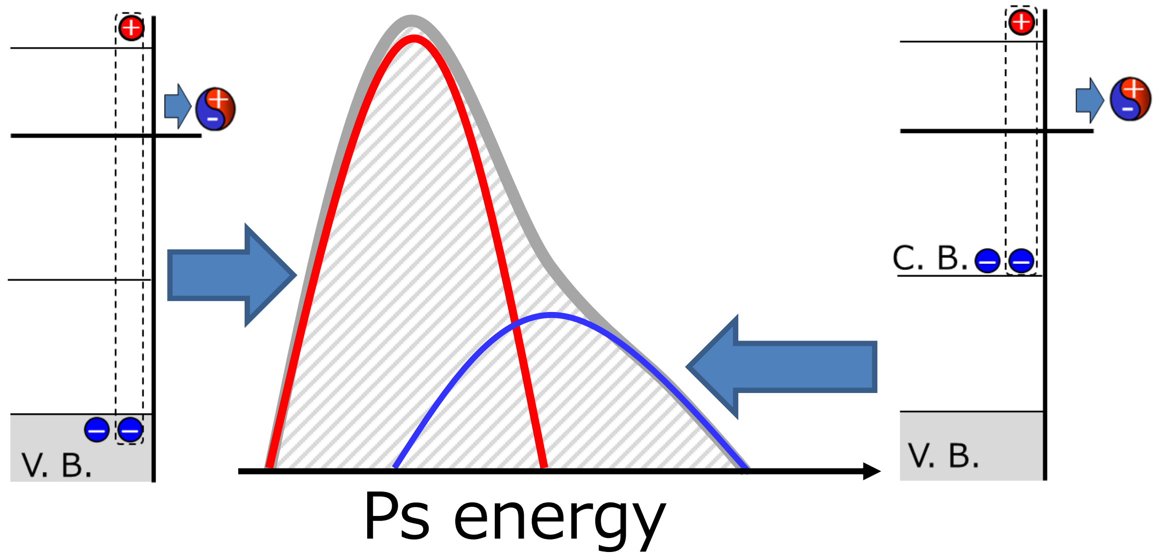
Two Ps components are found :
(I) Valence electrons,
(II) Excited states above valence band.



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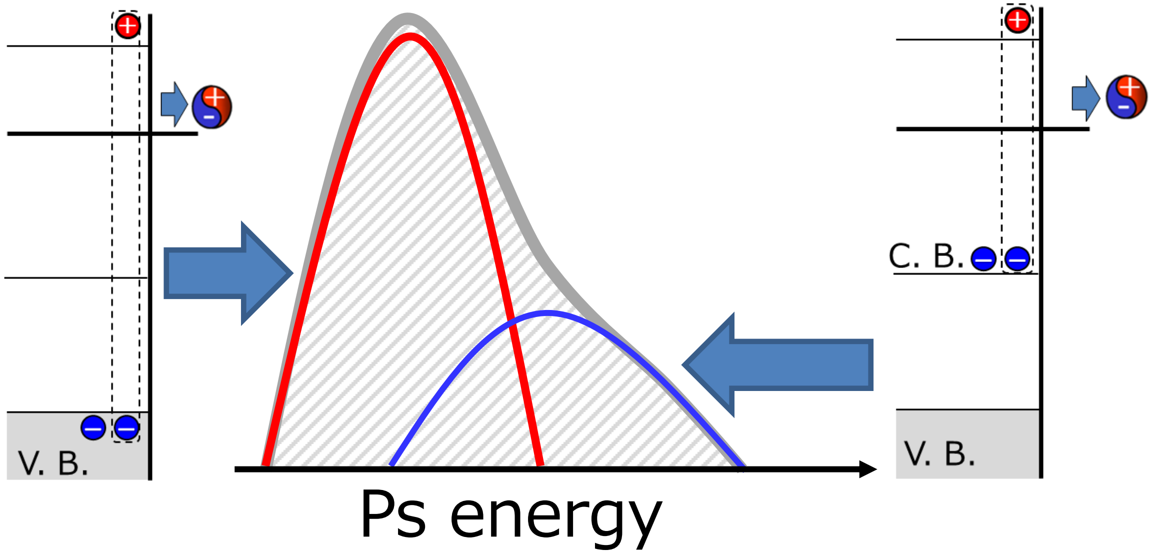

Ps TOF spectroscopy is effective to study Ps energy distribution.

Summary and prospects

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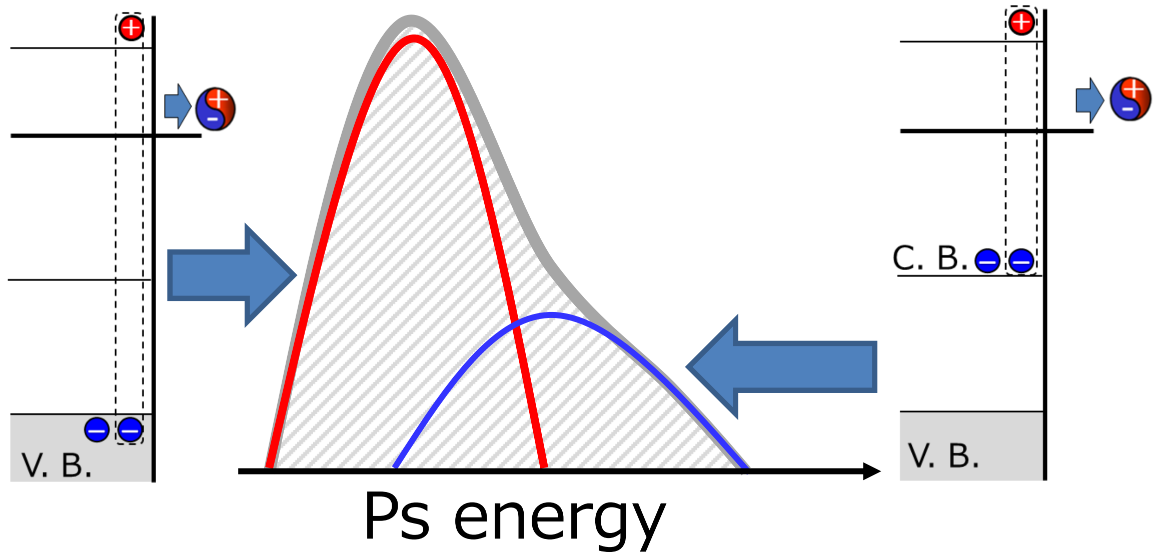
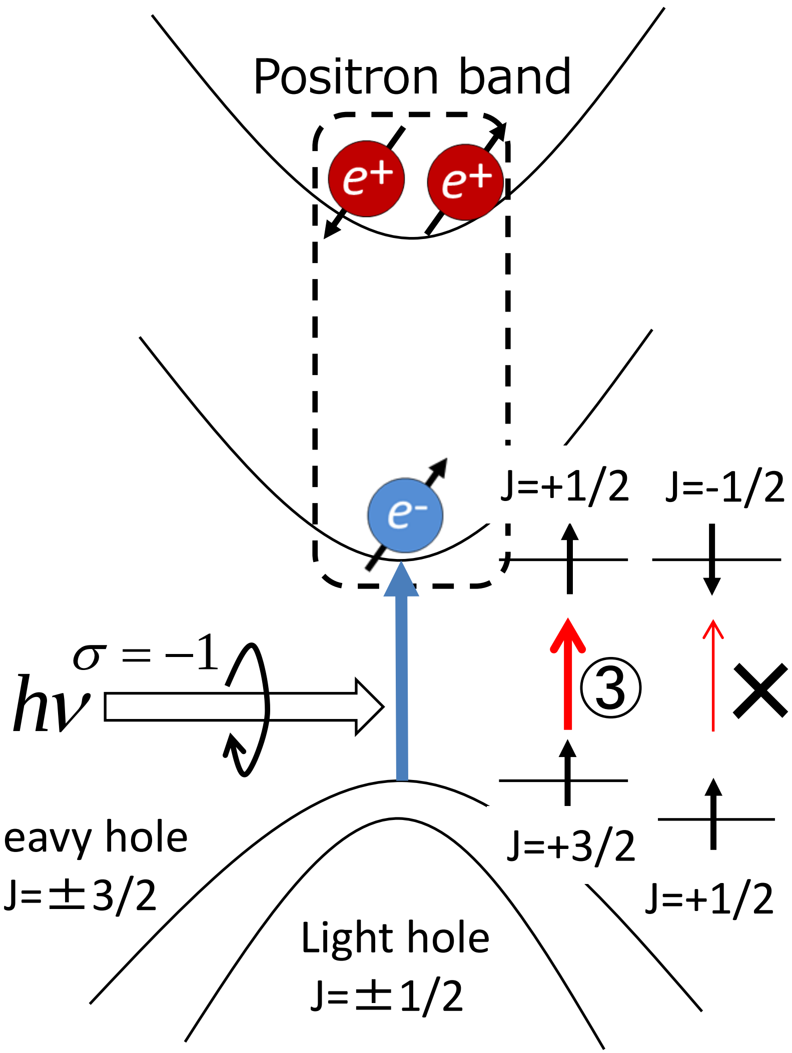
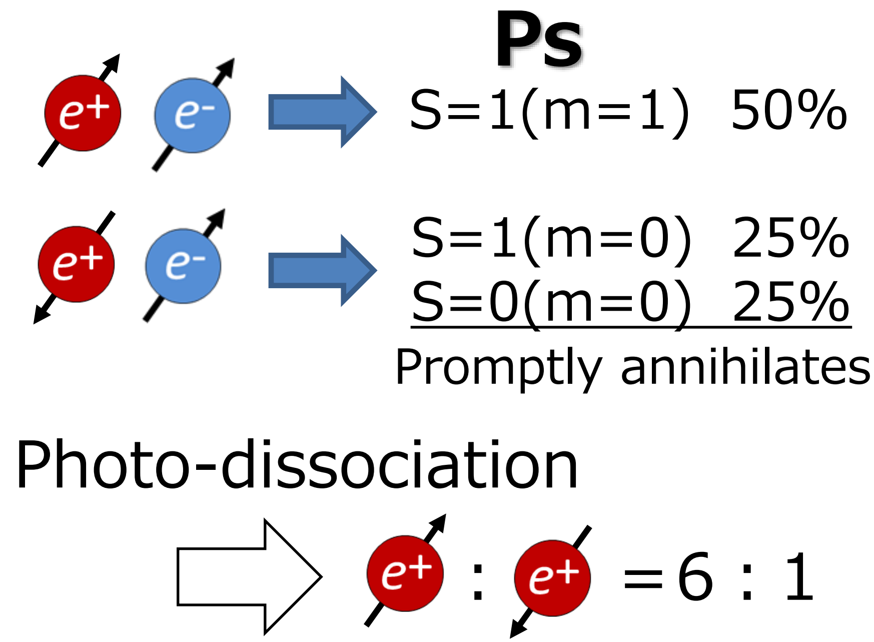


Ps TOF spectroscopy is effective to study Ps energy distribution. However, for more precise arguments including angle distribution, some new methods need to be developed.

Summary and prospects

Ps emission via excited electron state
→Application to Positron Spin Filter?





Spin polarization～70%