Quelle: Chem. Soc. Rev. 38 (2009)

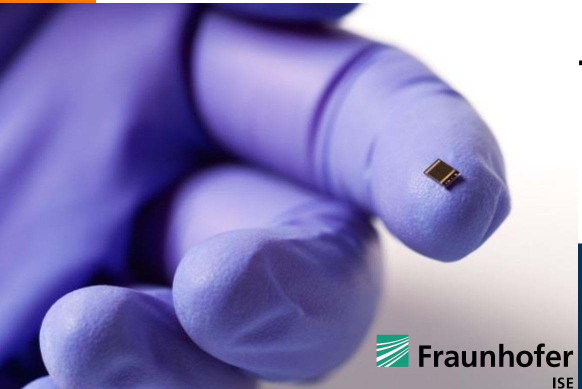
Multi junction concepts for photovoltaics and artificial photosynthesis:

Critical points of current and future high-performance solar energy conversion

T. Hannappel

Technische Universität Ilmenau,

Dep. of Photovoltaics



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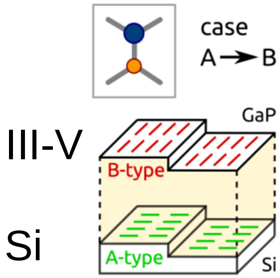
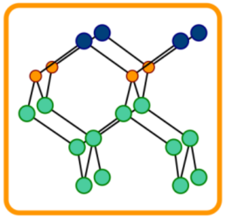
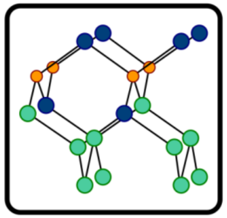
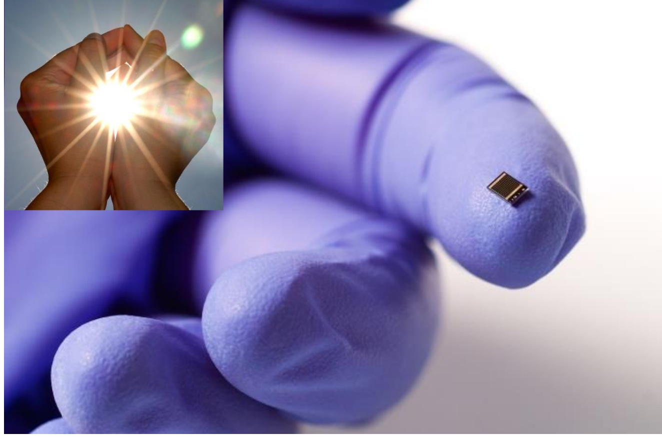








1. Record cell development

Fraunhofer ISE
Soitec
cea tech

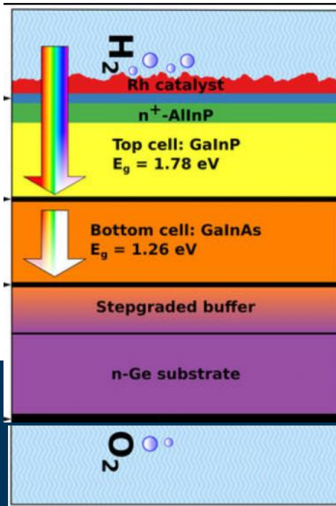
Highest efficiencies for solar cells and solar H-production:

HZB Helmholtz Zentrum Berlin

- 46 % in photovoltaics
- 14 % in direct solar-to-H-generation

JCAP JOINT CENTER FOR ARTIFICIAL PHOTOSYNTHESIS

2. Interfaces, III-V and Si(100) – a highly attractive couple

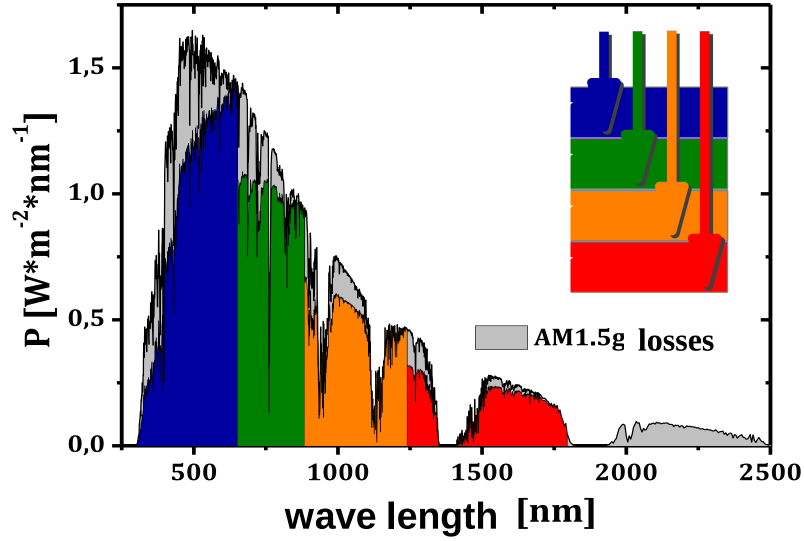


- Atomic scale analysis and control of defect-free nucleation

Critical points

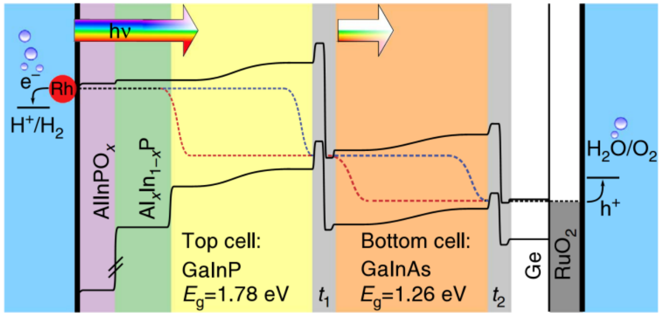
➢ **Physics:**

3rd generation PV,
only type demonstrated to exceed Shockley-Queisser limit



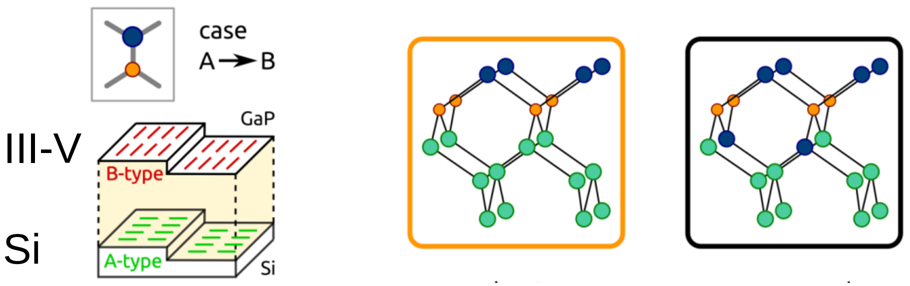
➢ **Chemical physics:**

Maximizing chemical potentials, interfacial reactions



➢ **Materials science:**

Atomic scale control, III-V semiconductors



➢ **Further aspects:**

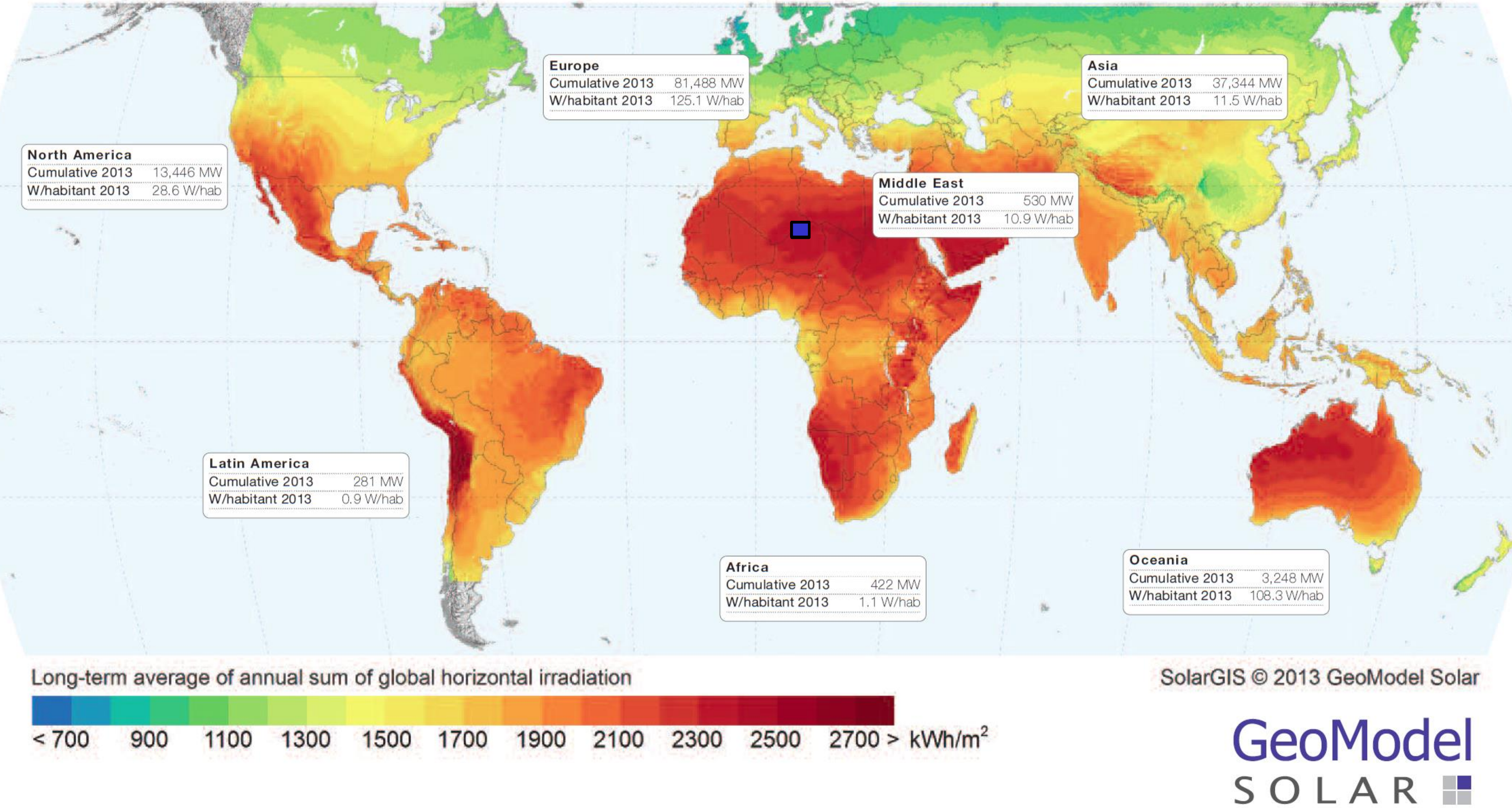
Optical management and more

Humanity's Top Ten Problems for next 50 Years

1. ENERGY
2. WATER
3. FOOD
4. ENVIRONMENT
5. POVERTY
6. WAR
7. DISEASE
8. EDUCATION
9. DEMOCRACY
10. POPULATION

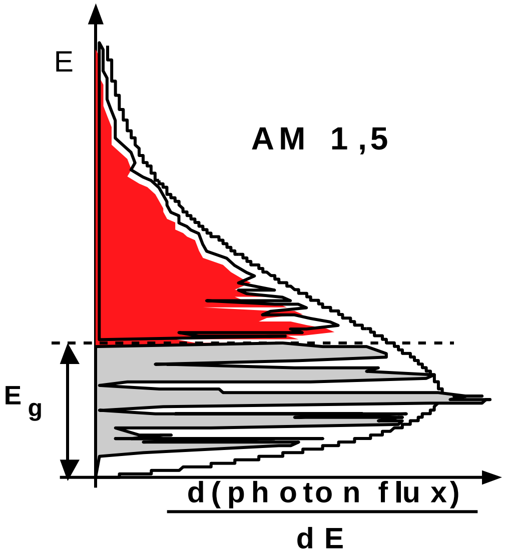
Source: Prof. R.E. Smalley, "Our Energy Challenge", Colombia University, NYC, 23 September 2003

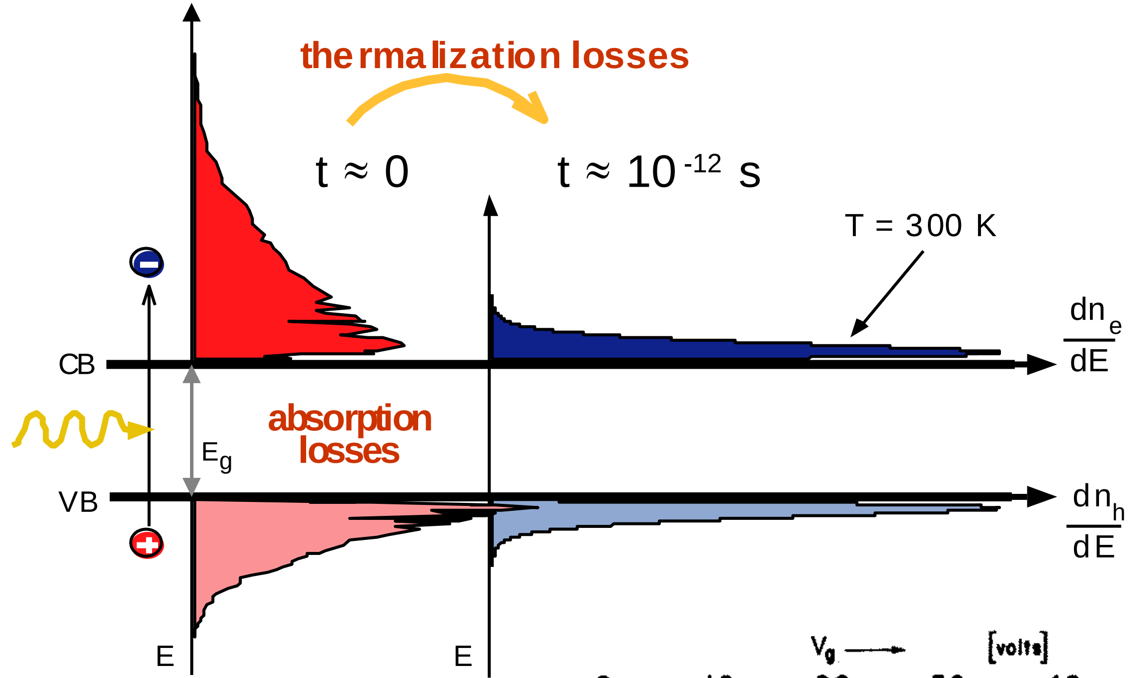
Global PV regional installations per habitant

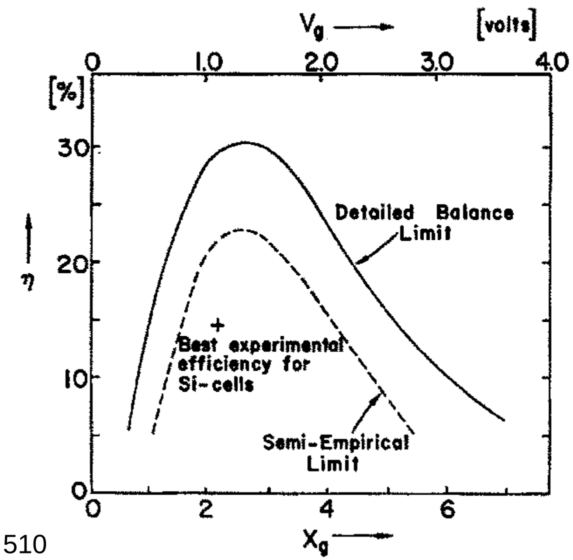


Source: EPIA, European PV Industry Association

Inherent losses in a single junction absorber







thermodynamic limits (radiative recombination only):

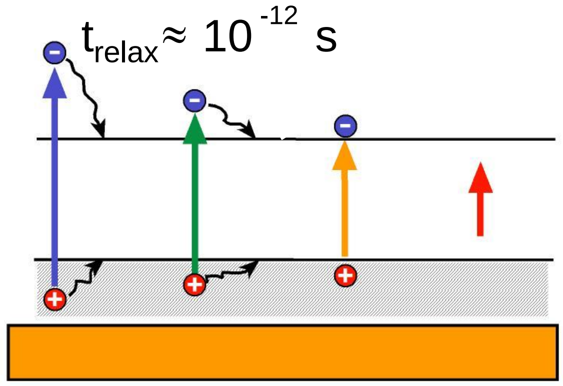
single junction ~ **30 (44)%**

optimum system ~ **66 (86)%**

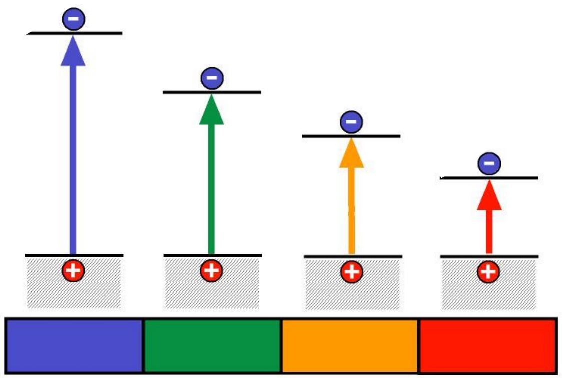
Shockley, Queisser, J. Appl. Phys. 32 (1961) 510

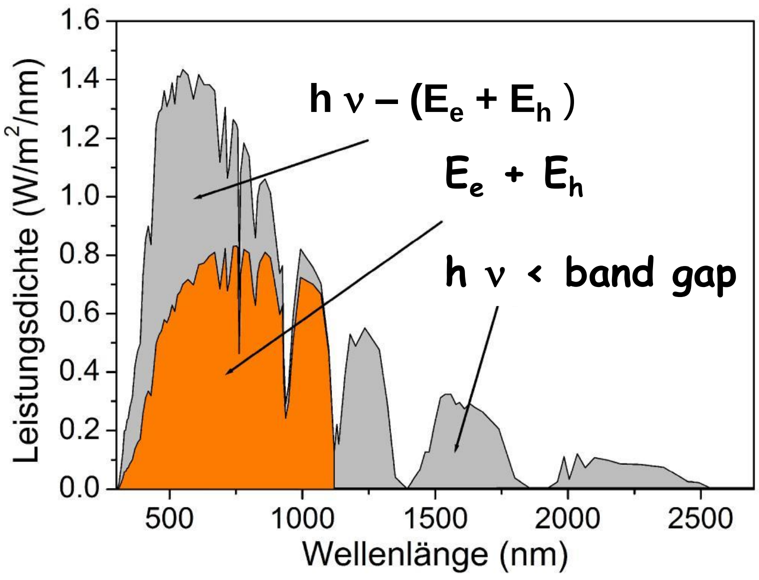
Reducing losses: 3rd generation photovoltaics

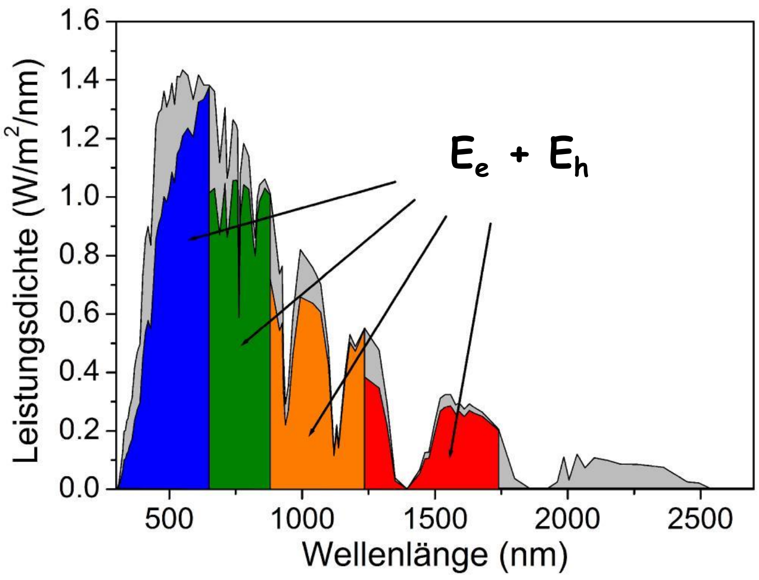
Single junction



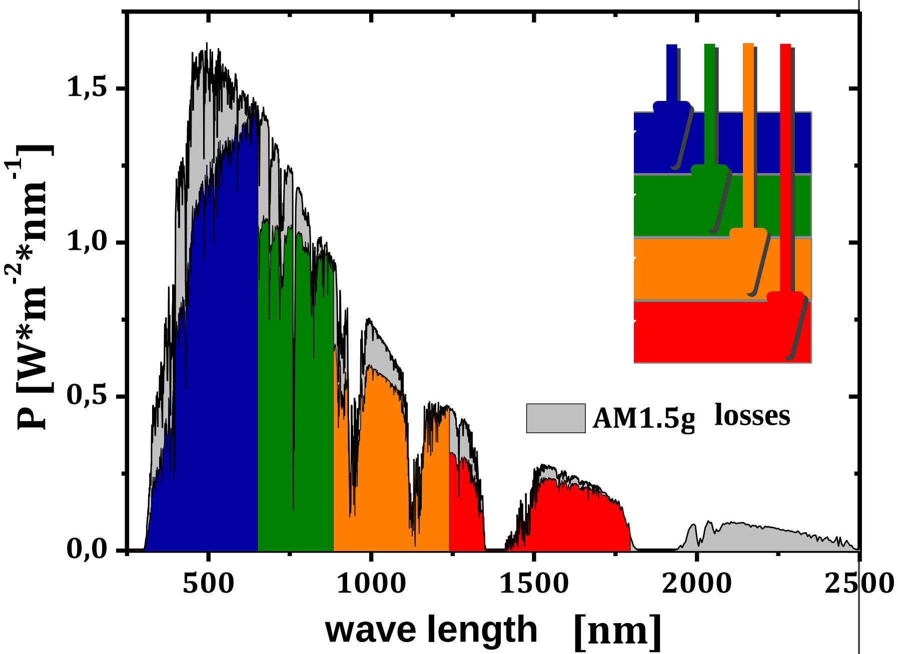
Multi junction

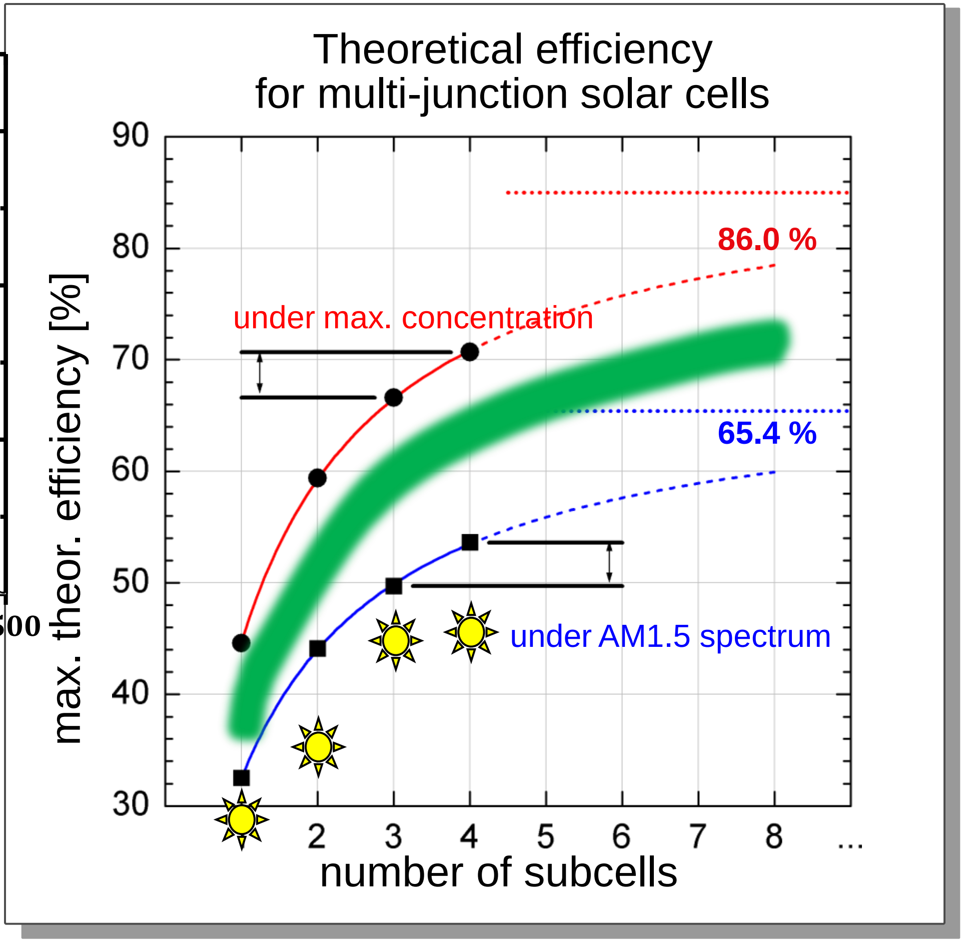






Theory: Multi junction solar cells & concentration C





Concentration C

$P_{SC} \propto I_L V_{OC} \propto C \ln C$
$\eta \propto \ln C$
$C_{max} \cong 46200$

$$V_{OC} = \frac{kT}{e} \ln\left(\frac{I_L}{I_0} + 1\right)$$

C: sun concentration

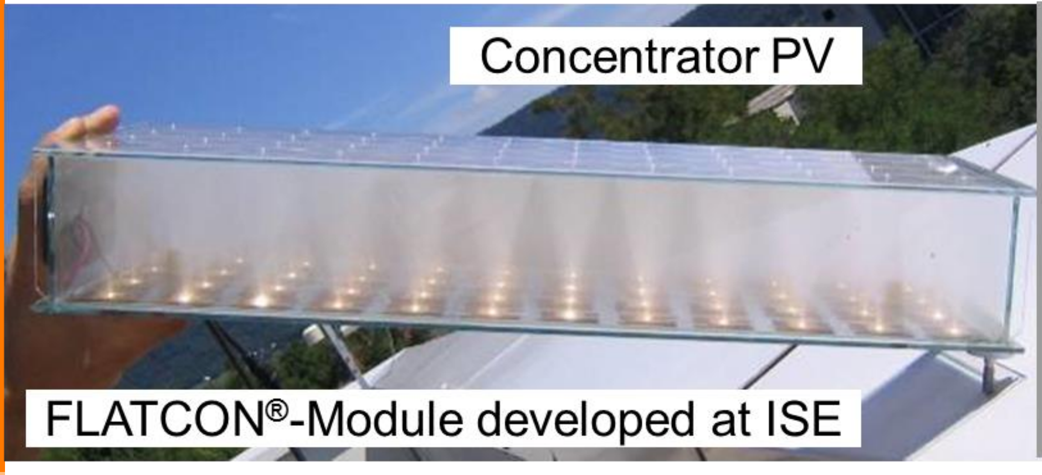
best values currently:

1 junction: 29.1%
2 junction: 34.1%
3 junction: 44.4%
4 junction: 46.0%

Shockley, Queisser, J. Appl. Phys. 32 (1961) 510

Photovoltaics:
Standard PV / Concentrator PV

light collection
and
conversion
is one unit

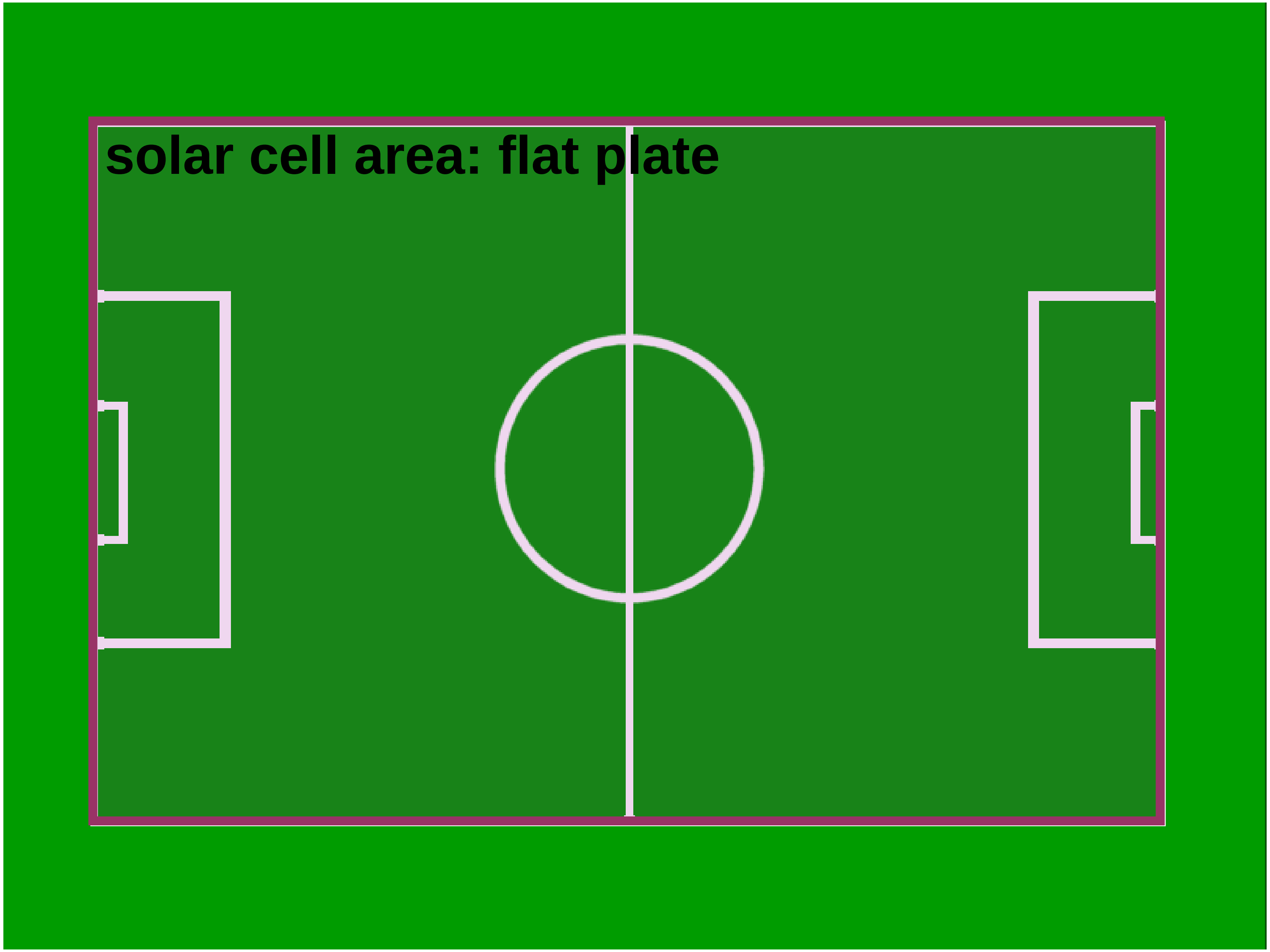


light collection
collection area

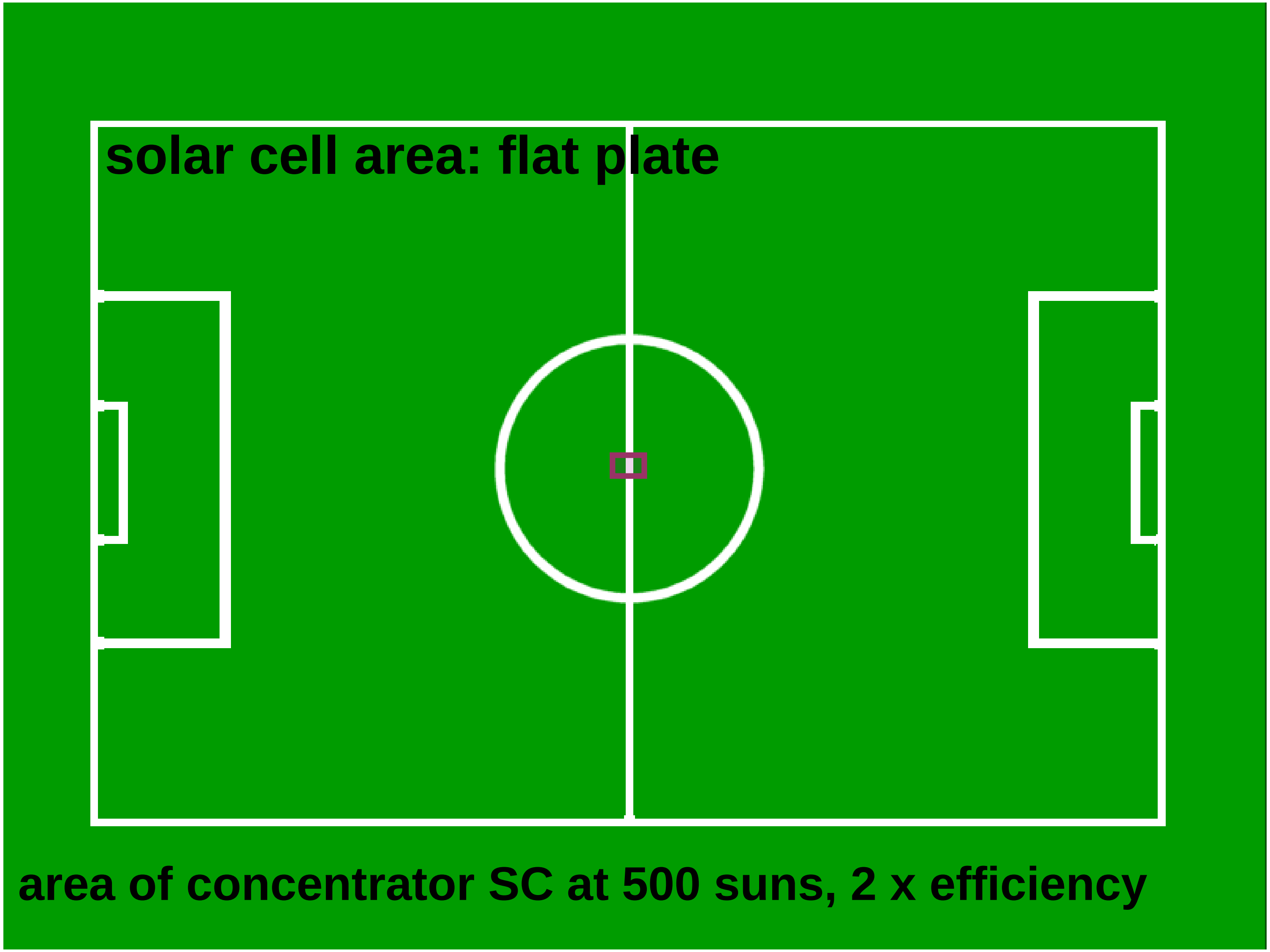
separated from

light conversion
cell area

concentration factor = collection / cell area


solar cell area: flat plate

Concentrator photovoltaics - solar cell area



source: FhG ISE

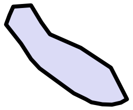
Soitec Solar, Touwsrivier, South Africa

Soitec

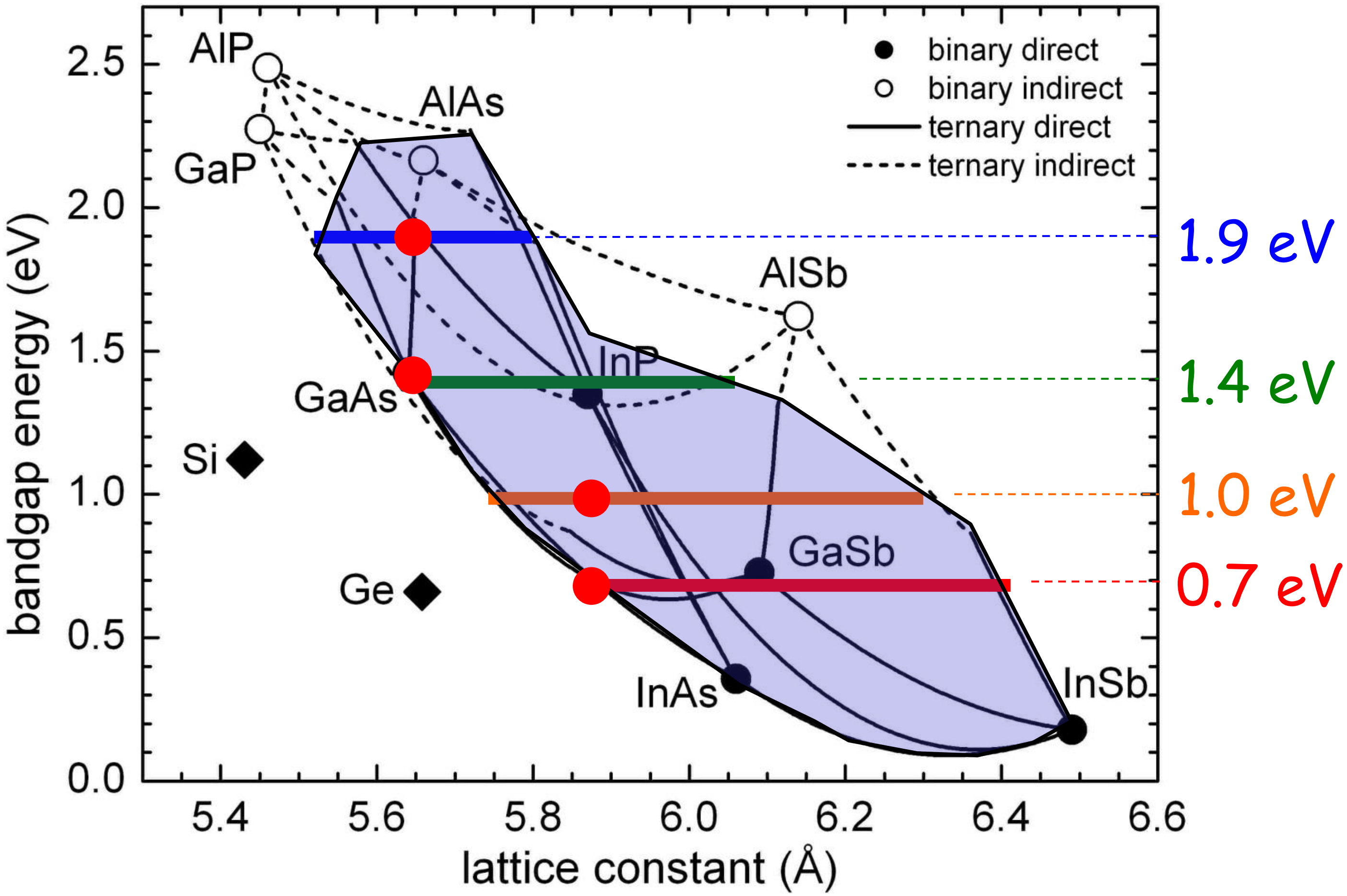
44 MWp capacity, projected in South Africa

Concentrator Photovoltaic (CPV) –
Largest HCPV-Installation Site: Golmud, China

Optimum bandgaps for a 4-junction solar cell –
problem: lattice-mismatch causes defects



direct band gaps



Solution: wafer bonding

Four-junction solar cell under concentrated sunlight via wafer bonding

$\eta = 44.7\ \%$

at 297 suns

F. Dimroth, M. Grave, …, T. Hannappel, K. Schwarzburg, Prog. Photovolt: Res. Appl. 22 (2014) 277

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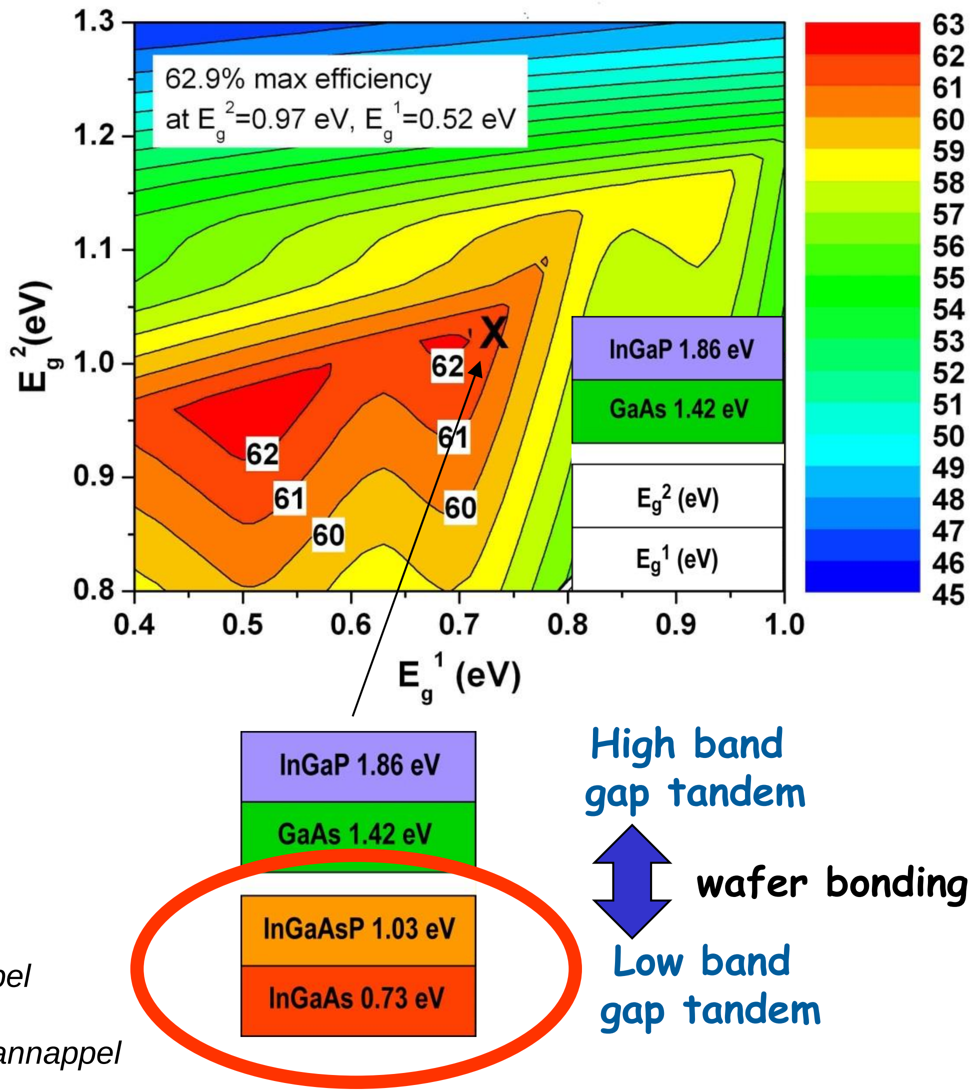
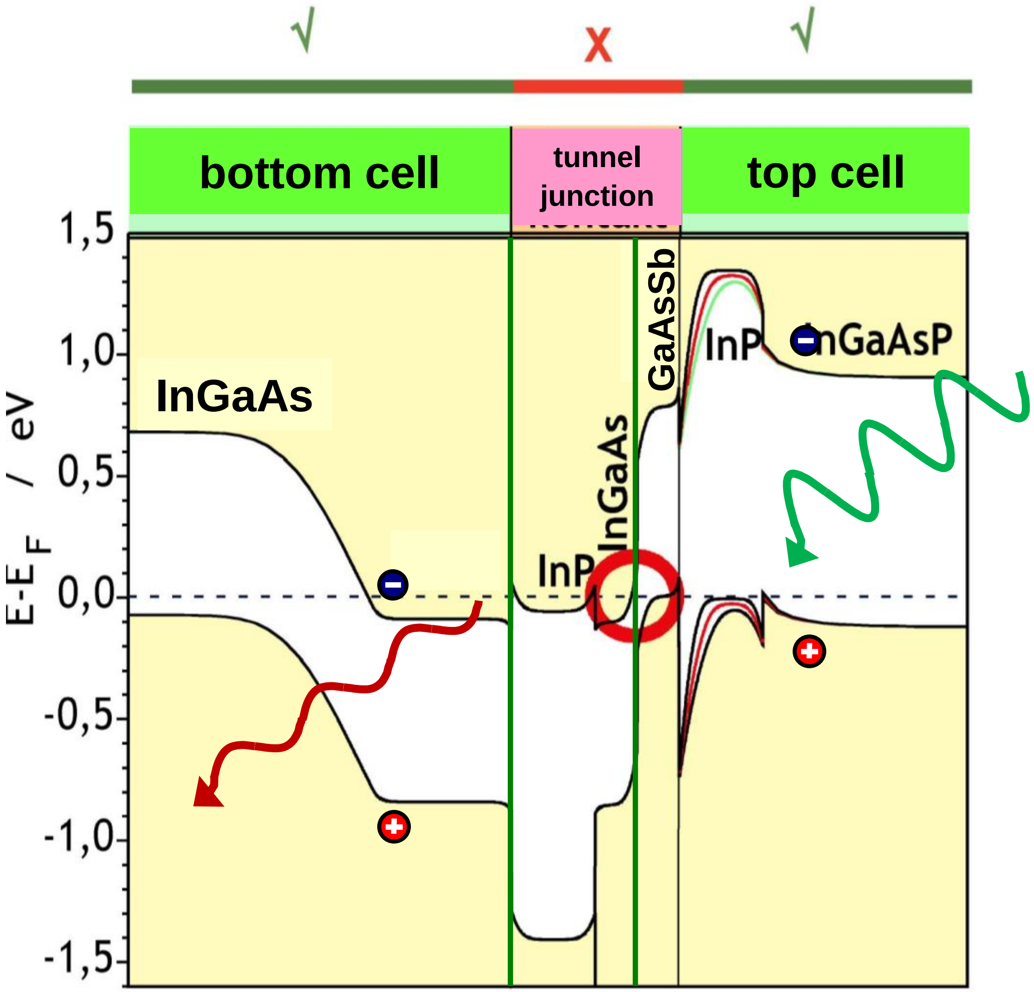


B.E. Sağol, U. Seidel, … , K. Schwarzburg, T. Hannappel Chimia 61 (2007) 775
N. Szabo, B.E. Sağol, U. Seidel, K. Schwarzburg, T. Hannappel phys. stat. sol. – RRL 2 (2008) 254

Tandem cell: tunnel junction, current matching, …



top cell		InGaAsP	2 µm
BSF	p	InP	50 nm
tunnel	p++	GaAsSb	15 nm
contact	n++	InGaAs	15 nm
barrier	n+	InP	[illegible]0 nm
bottom cell		InGaAs	3 µm

Sağol, Seidel, … , Schwarzburg, Hannappel
Chimia 61 (2007) 775
Szabo, Sağol, Seidel, Schwarzburg, Hannappel
phys. stat. sol. – RRL 2 (2008) 254

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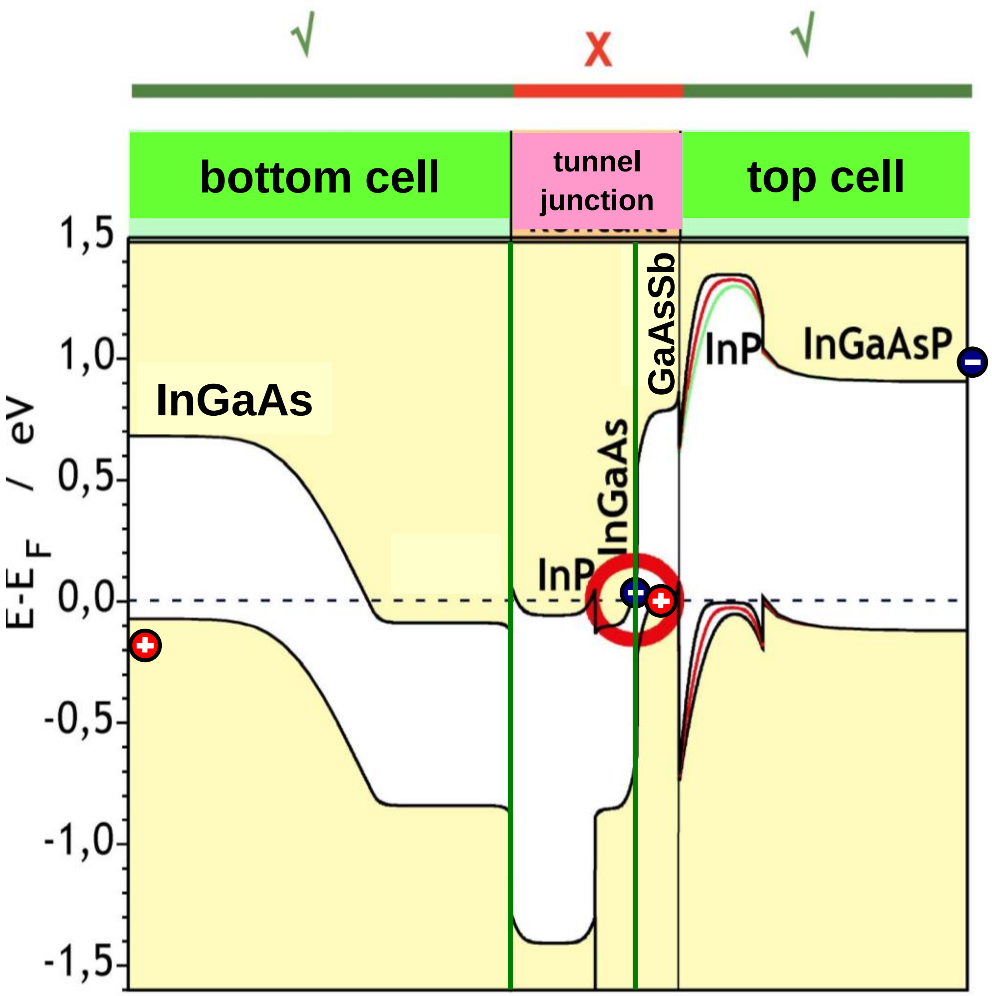
Thomas Hannappel
DPG

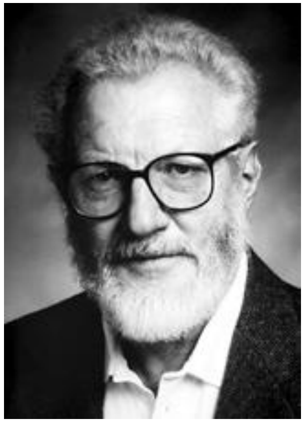
Tandem cell: tunnel junction, current matching, …



top cell		InGaAsP	2 µm
BSF	p	InP	50 nm
tunnel	p++	GaAsSb	15 nm
contact	n++	InGaAs	15 nm
barrier	n+	InP	30 nm
bottom cell		InGaAs	3 µm

Interfaces

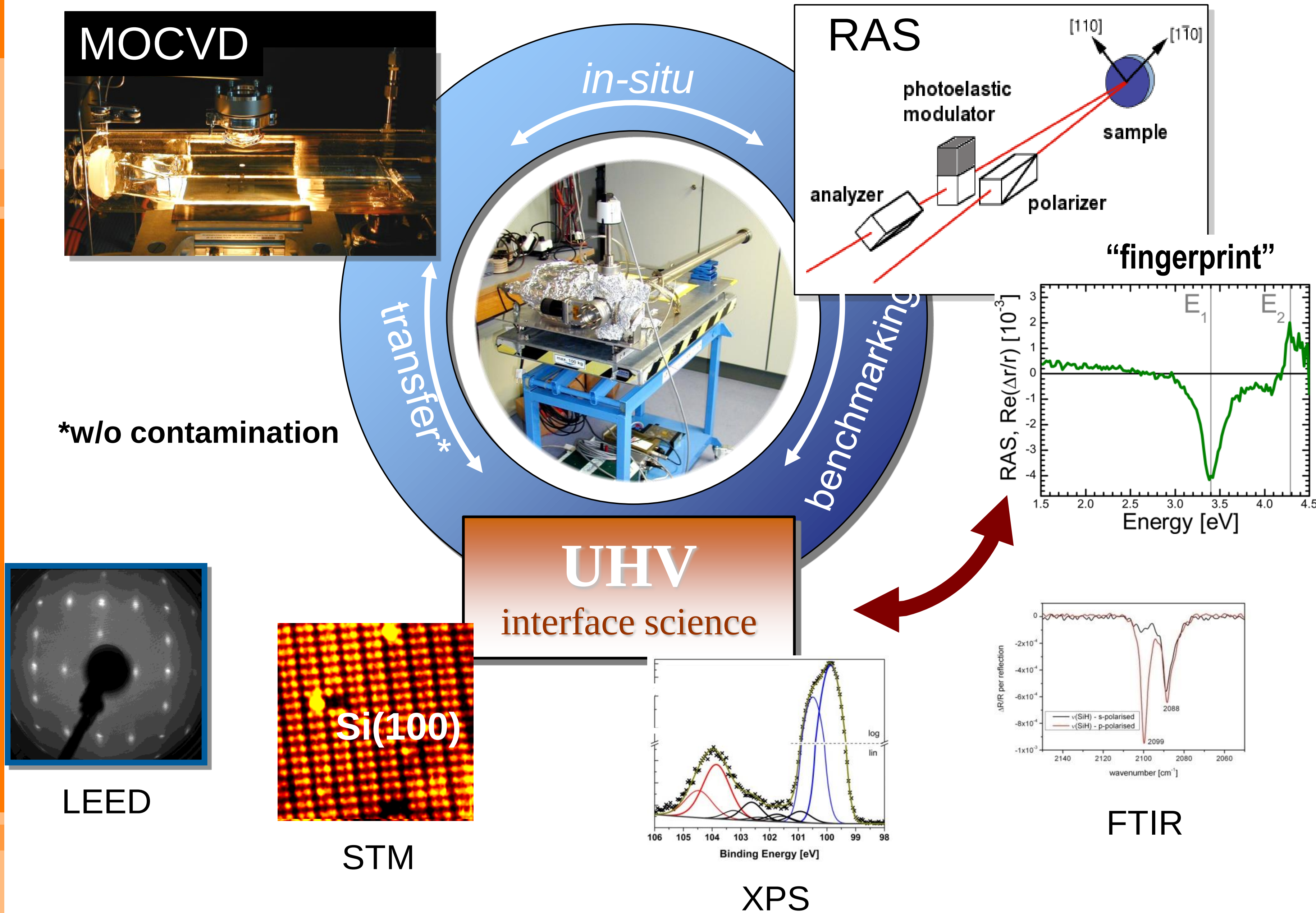
"Heterostructures, as I use the word here, may be defined as heterogeneous semiconductor structures built from two or more different semiconductors, in such a way that the transition region or interface between the different materials plays an essential role in any device action. Often, it may be said that *the interface is the device.*"



Herbert Krömer, German Physicist and Nobel laureate („For developing semiconductor heterostructures used in high-speed- and opto-electronics "), 2000

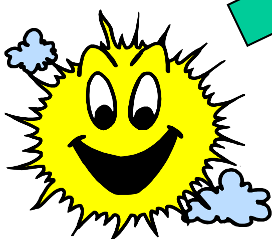
""God created solids,
but surfaces were the work of the devil"

Wolfgang Ernst Pauli (* 25. April 1900 in Wien; † 15. Dezember 1958 in Zürich), one of the most significant physicist of the 20th century and Nobel laureate.

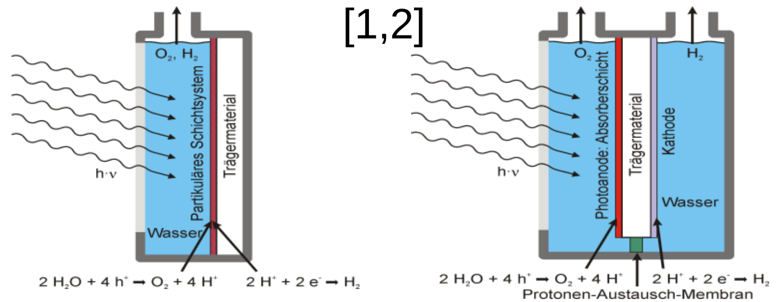


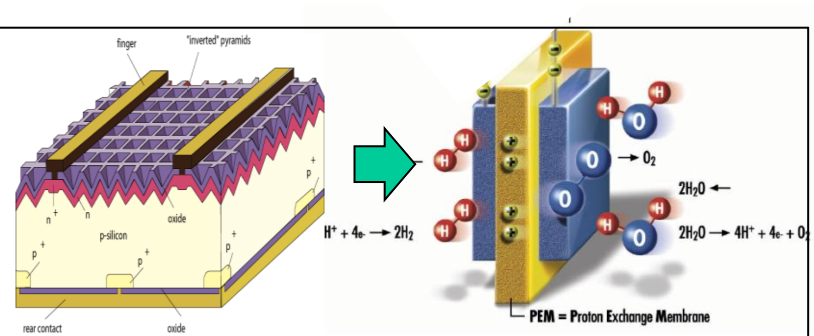
T. Hannappel et al.,
Rev. Sci. Instr. 75 (2004) 01297
German patent (1999) DE 19837851

Routes to generate solar fuels (H_2, methane, …)

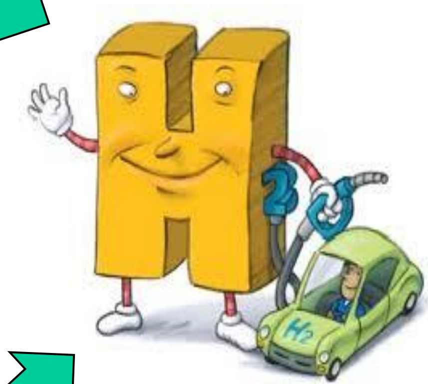


Photocatalysis and Photoelectrochemistry [1,2]



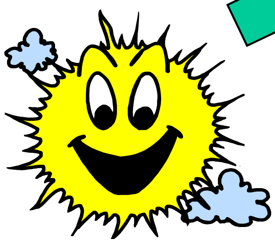


Solar cell plus electrolyser [3]

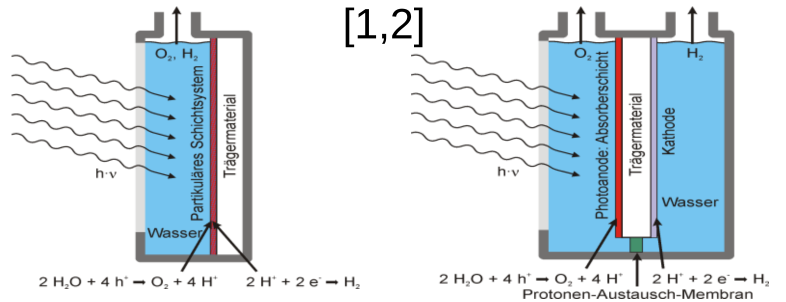


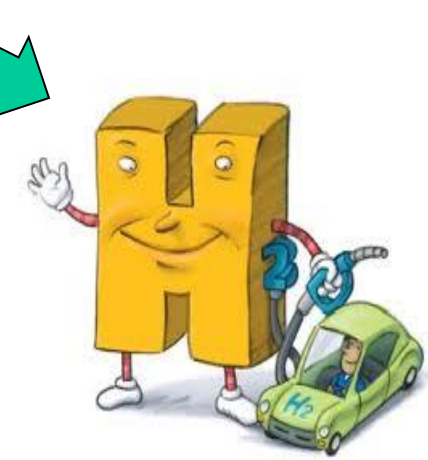
[1] Cook, …, Nocera, *Chem. Rev.* **110** (2010), [2] May, …, Hannappel, *Nature Comm. (2015),*
[3] Luo, …Grätzel, *Science* **345** (2014).

Routes to generate solar fuels   (H_2, methane, …)



Photocatalysis and Photoelectrochemistry [1,2]

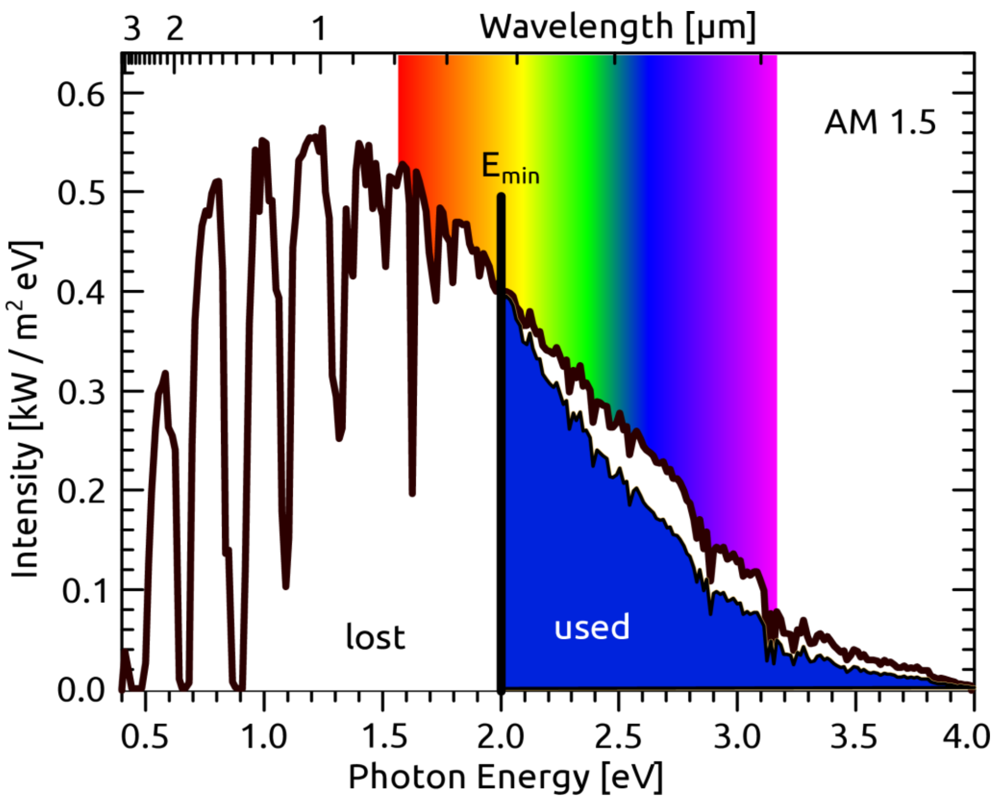


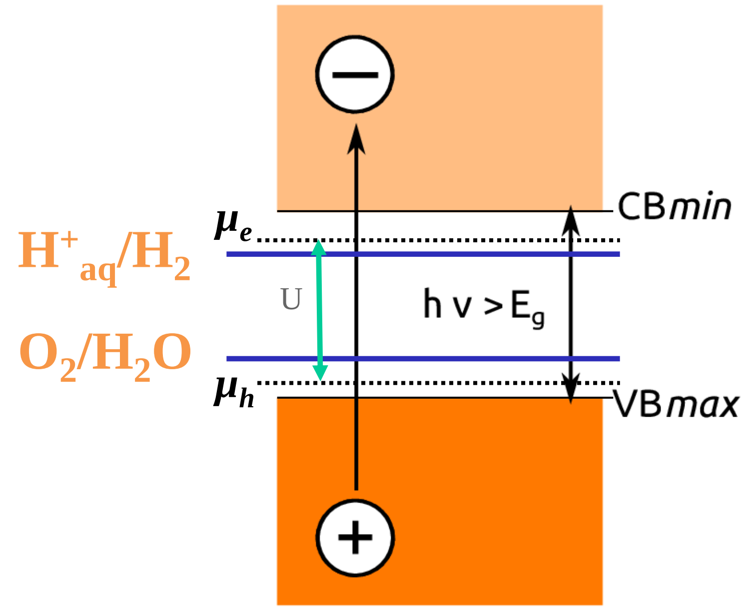


[1] Cook, …, Nocera, *Chem. Rev.* **110** (2010), [2] May, …, Hannappel, *Nature Comm. (2015)*

Tandems for unassisted water photolysis

bias-free solar watersplitting needs energy gap > 2eV





$$\mu_i = \mu_{i,0} + kT \ln\left(\frac{n_i}{N_i}\right)$$

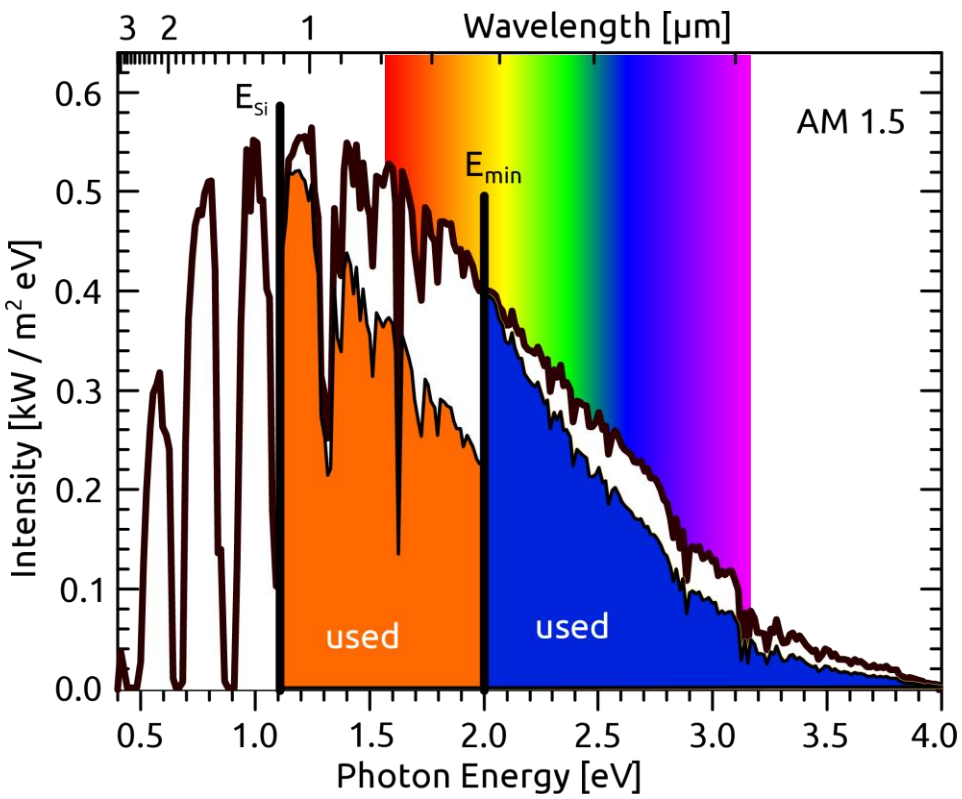
under illumination

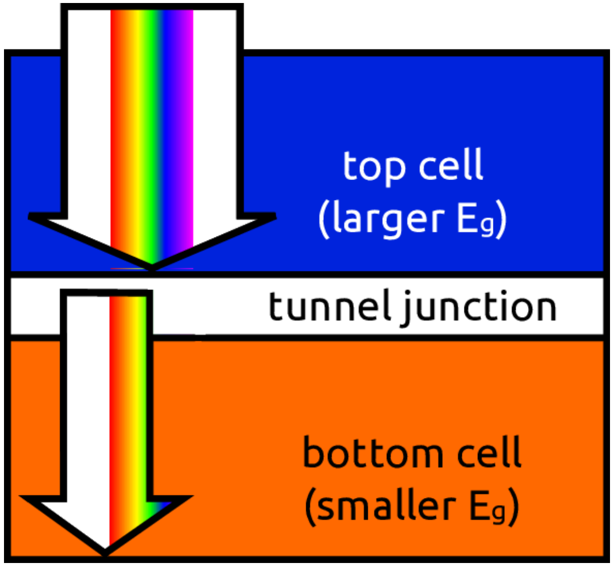
$$\mu_e + \mu_h = \varepsilon_{FC} - \varepsilon_{FV}$$

T. Hannappel, M.M. May, H.J. Lewerenz, chapt. 9 *in: Photoelectrochemical Water Splitting: I ssues & Perspectives* **RSC Publishing**, Energy and Environment Series (2013)

Tandems for unassisted water photolysis

solar exploitation → tandem



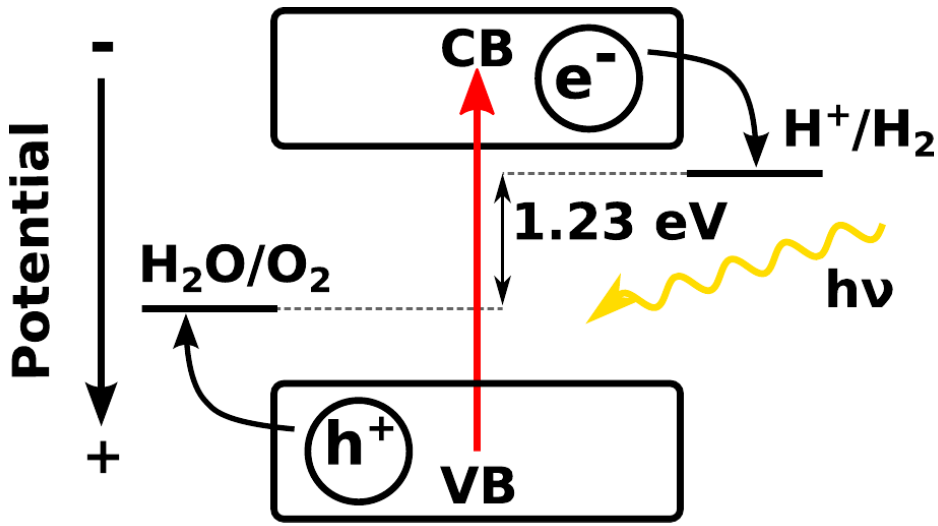


→ current matching

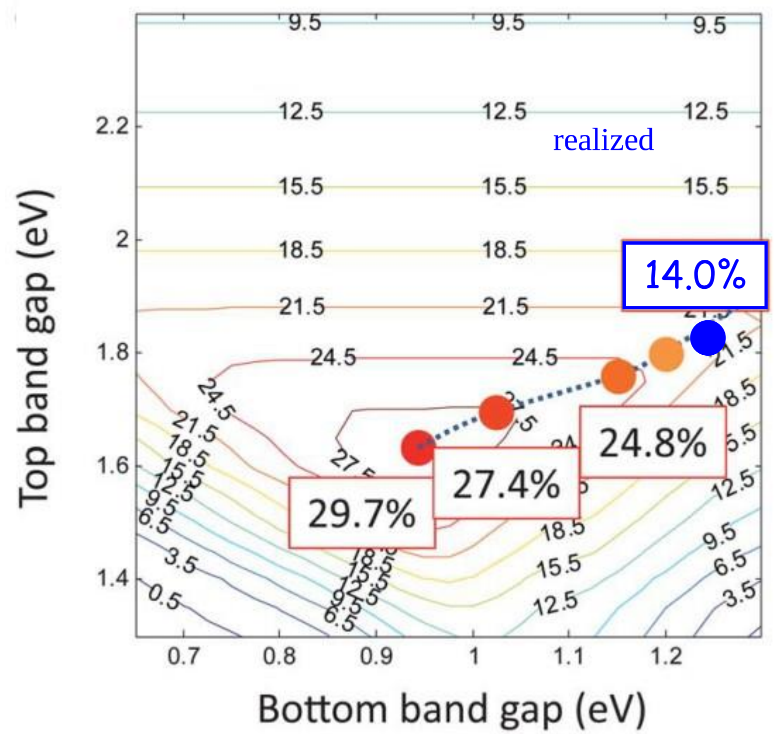
Potential efficiencies of tandems for water-splitting

- Bias-free solar watersplitting requires band gap > ca. 2.2 eV
- Beyond that: maximisation of the current

→ Tandems for efficiency optimum



Theoretical limits



Solar to hydrogen $$\eta = \frac{j_{H_2} \times 1.23\ \mathrm{V}}{P_{\mathrm{in}}/A}$$

S. Hu et al. *Energy Environ. Sci.* **6**:2984, 2013.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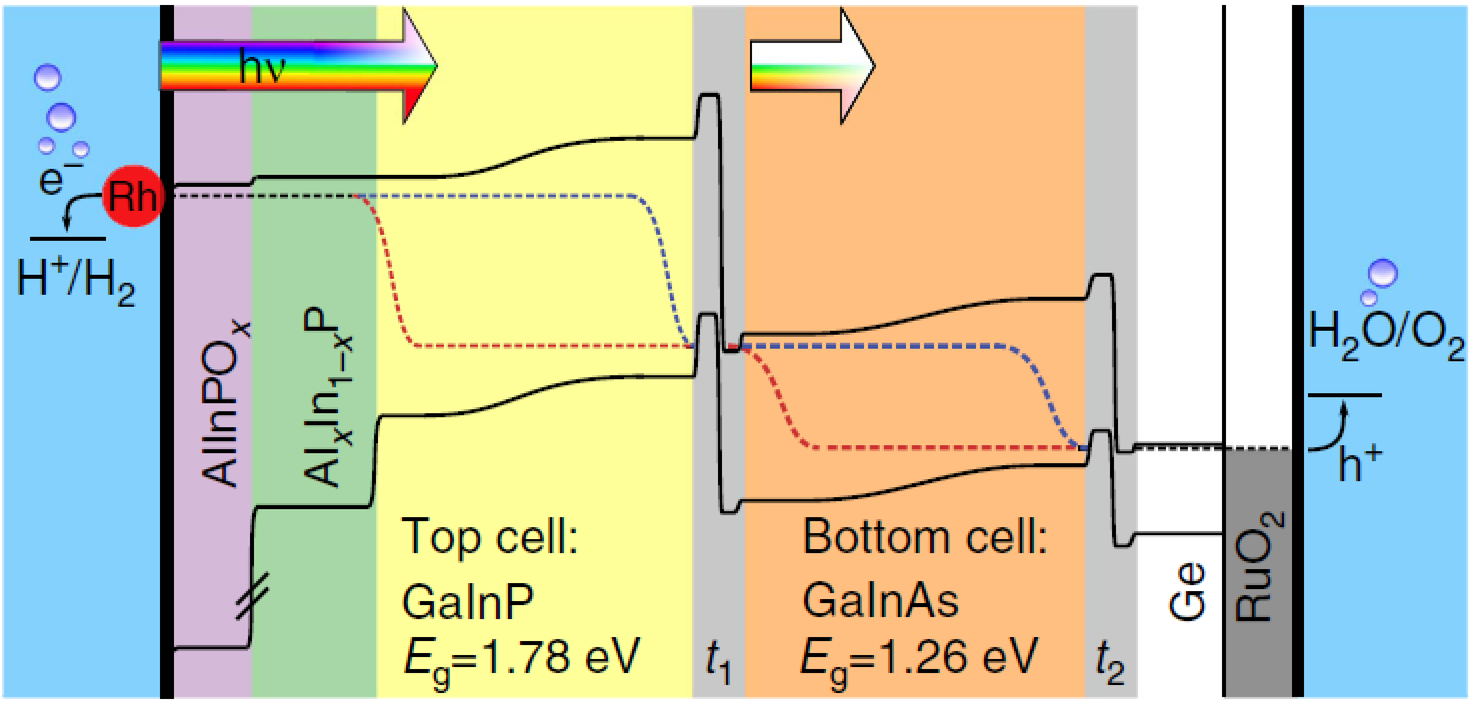
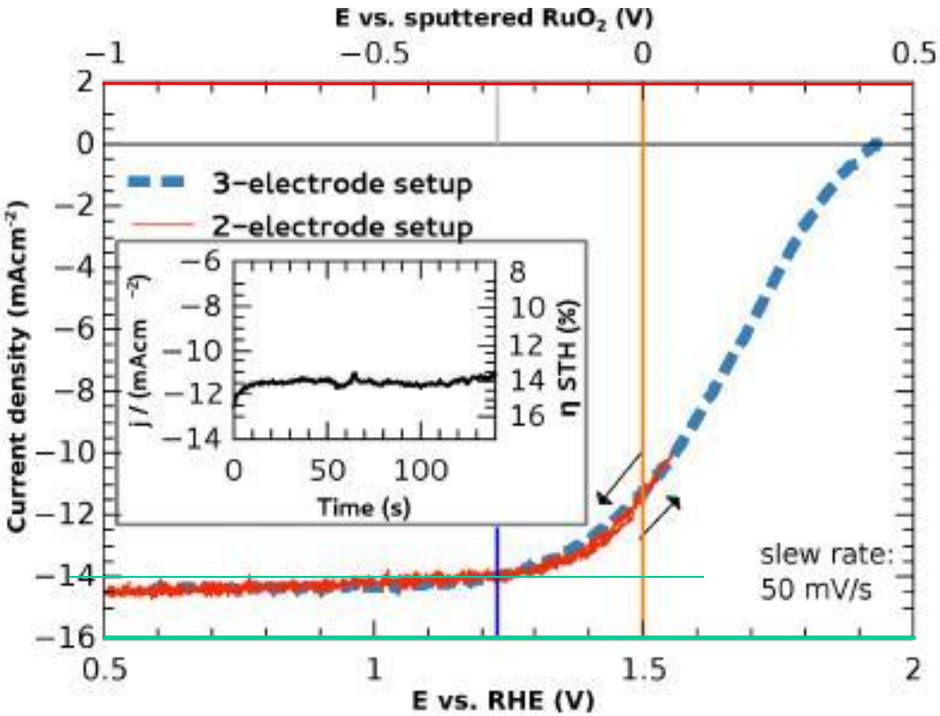
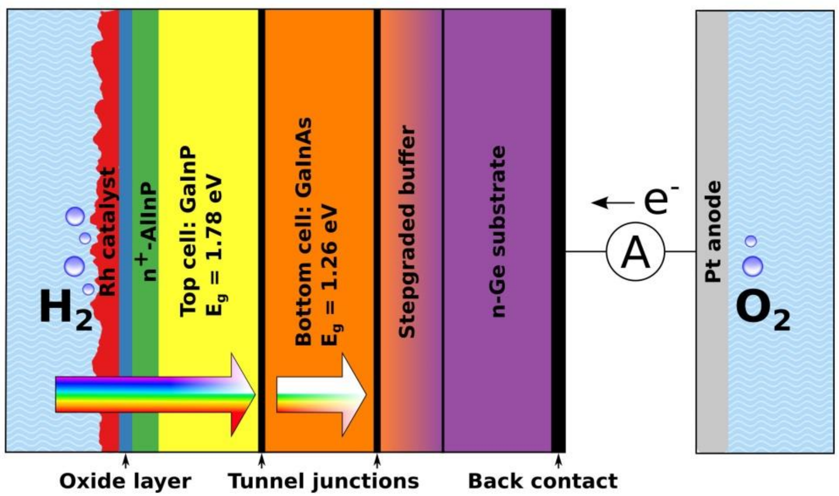
Energy schematic of the tandem layer structure
- under illumination



Monolithic 14 % water splitting tandem





- In situ functionalization of a III-V tandem

→ Rh electrocatalyst deposition & interface functionalization

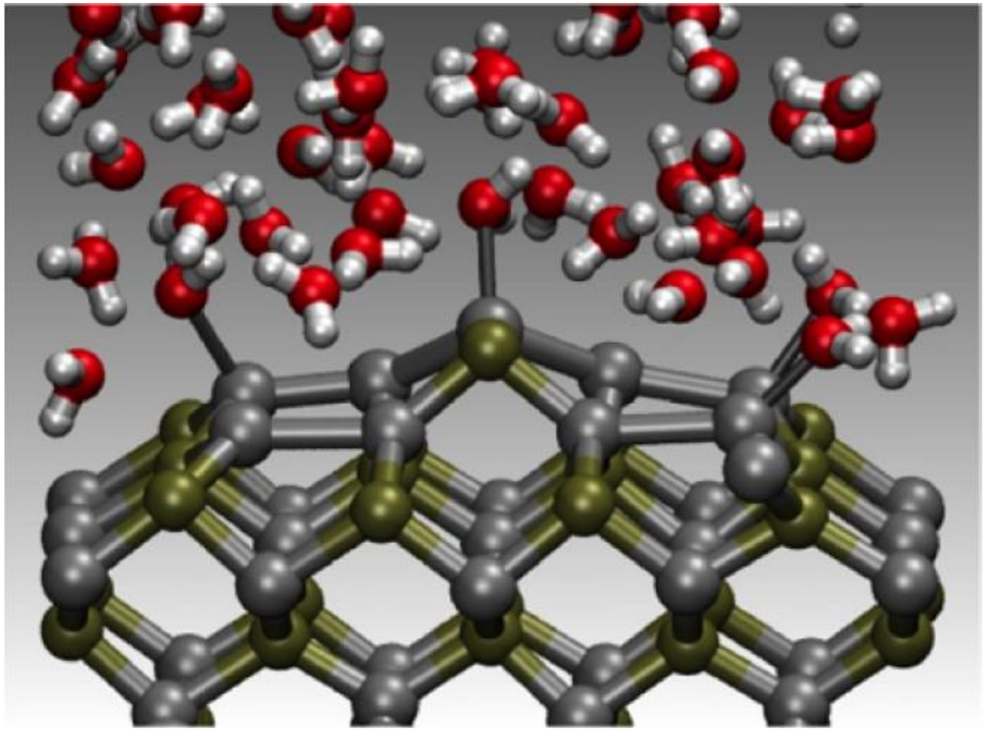
→ 14 % STH in a bias-free setup under AM 1.5G

M.M. May, H.-J. Lewerenz, D. Lackner, F. Dimroth, T. Hannappel, *Nature Comm. 6 (2015) 8256*

Study of liquid-solid interface

Theory + Experiment:

- Surface configuration impacts interaction with H_2O
- Metal–oxide–metal bonds affects charge transfer dynamics [1,2].

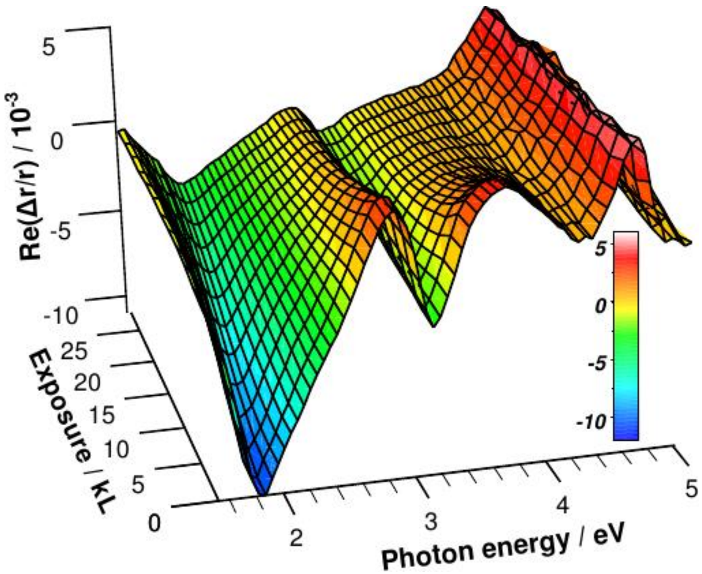


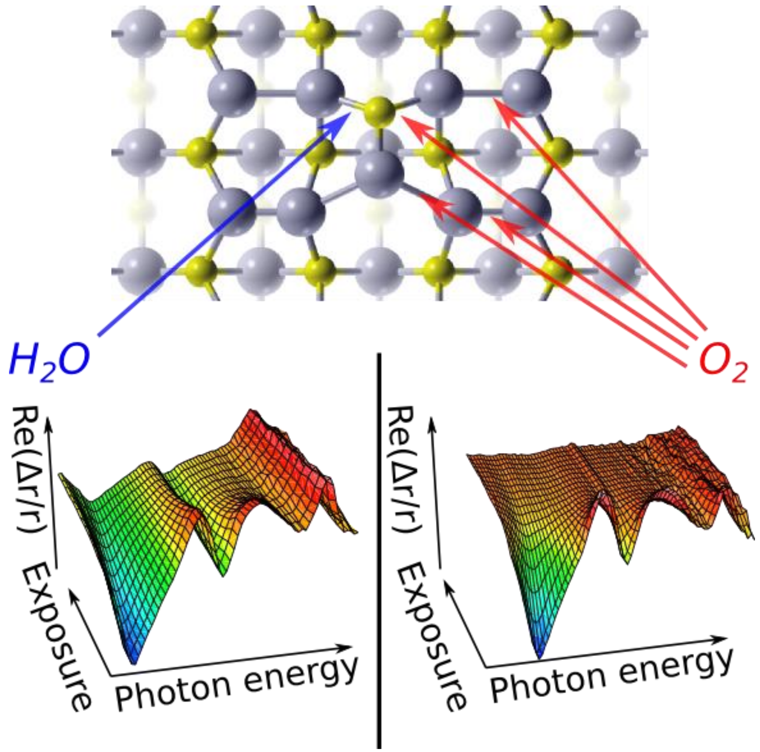
M.M. May, PhD thesis

[1] Wood et al., *J. Phys. Chem. C* **118** (2014).
[2] Kaiser et al., *ChemPhysChem* **13** (2012).

H_2O/O_2-adsorption on In-rich InP(100)

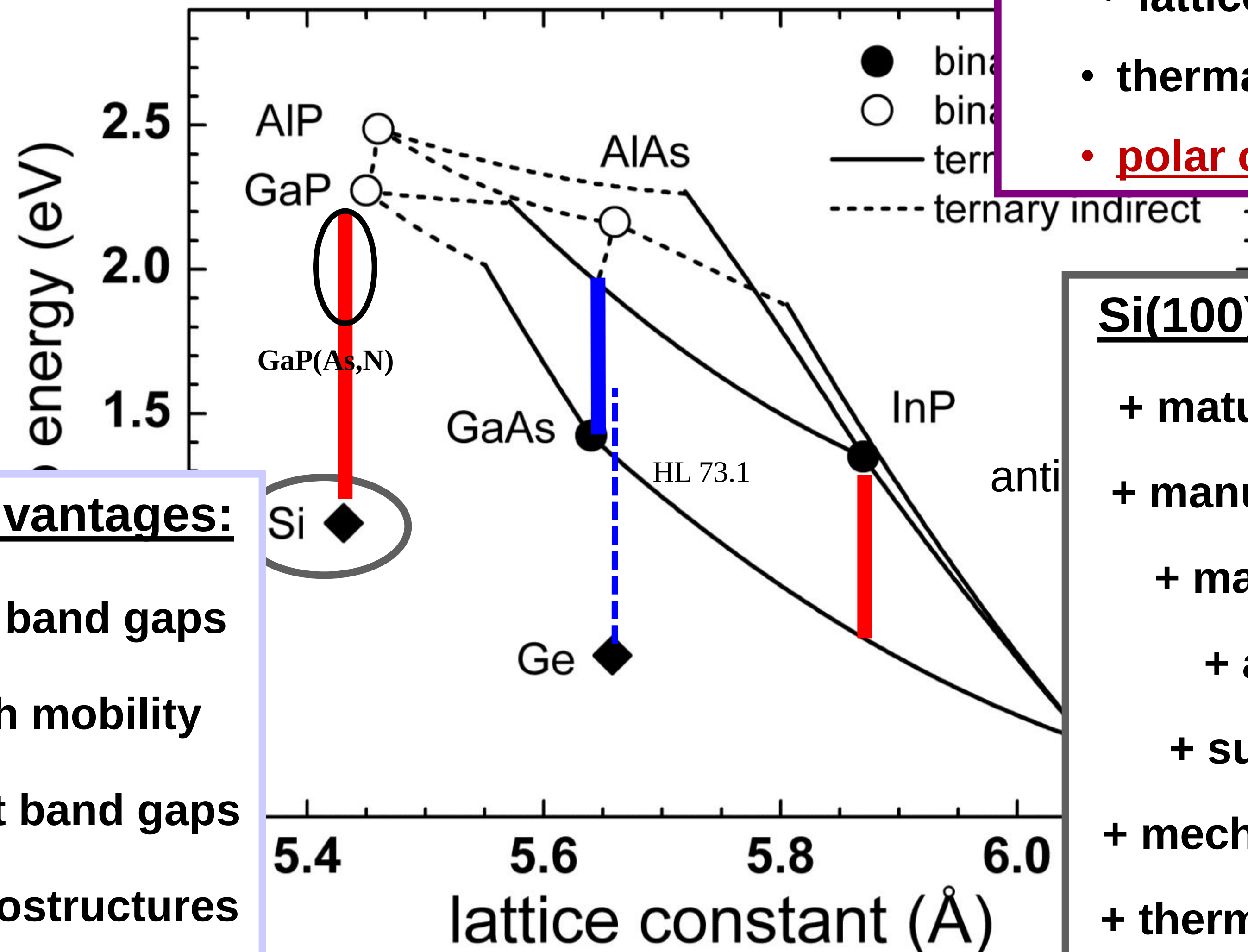
- In-rich InP(100) surfaces enable efficient & stable photocathodes [1]
- Exposure of well-defined InP(100) to water and oxygen
- In situ study of surface chemistry with RAS





[1] H-J Lewerenz, …, T.H., …, *En. Environ. Sci.* **3**:748 (2010).
[2] MM May, …, T.H., *J. Phys. Chem. C* **118**:19032 (2014).

III-V semiconductor heteroepitaxy on Si(100): potentials and issues



III-V on Si(100)

Epitaxial challenges:

- **lattice constants**
- **thermal expansion**
- **polar on non-polar**

III-V advantages:

+ high band gaps

+ high mobility

+ direct band gaps

+ heterostructures

+ MOVPE

+ optoelectronics

Si(100) advantages:

+ mature technology

+ manufacturing cost

+ material quality

+ availability

+ substrate size

+ mechanical integrity

+ thermal conductivity

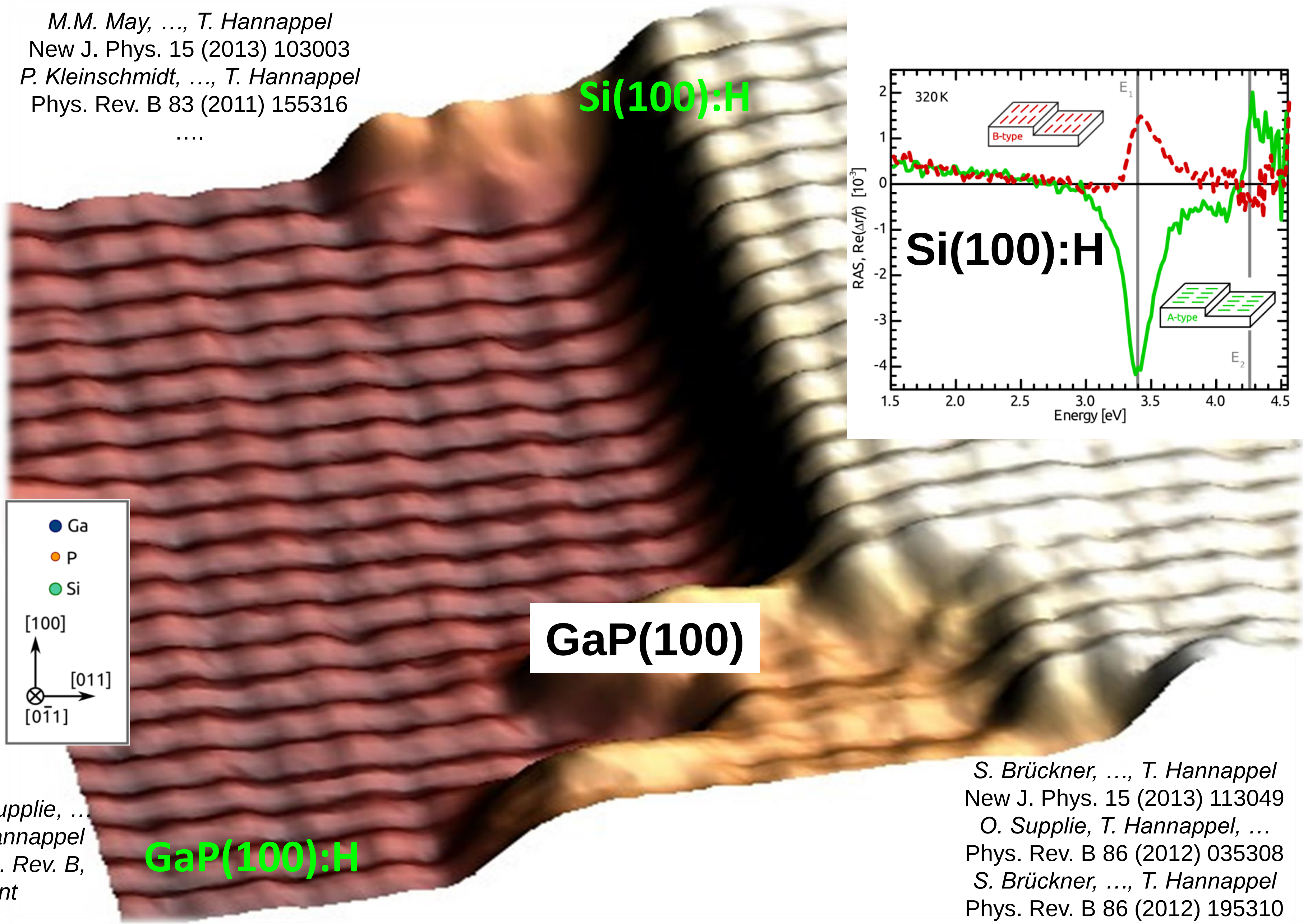
+ abundance

+ microelectronics

M.M. May, …, T. Hannappel
New J. Phys. 15 (2013) 103003
P. Kleinschmidt, …, T. Hannappel
Phys. Rev. B 83 (2011) 155316
….

III-V

Si



O. Supplie, …
T. Hannappel
Phys. Rev. B,
in print
….

S. Brückner, …, T. Hannappel
New J. Phys. 15 (2013) 113049
O. Supplie, T. Hannappel, …
Phys. Rev. B 86 (2012) 035308
S. Brückner, …, T. Hannappel
Phys. Rev. B 86 (2012) 195310
….

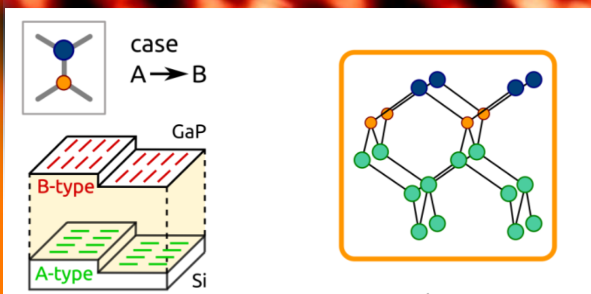
M.M. May, …, T. Hannappel
New J. Phys. 15 (2013) 103003
P. Kleinschmidt, …, T. Hannappel
Phys. Rev. B 83 (2011) 155316
….

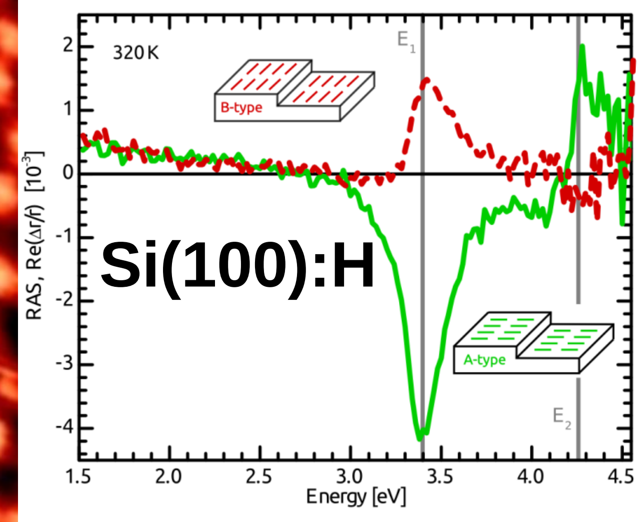
III-V

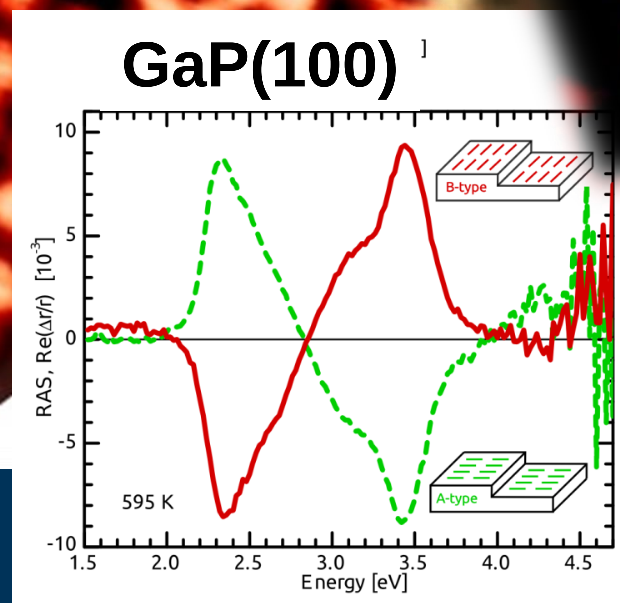
Si

Si(100):H

GaP(100):H



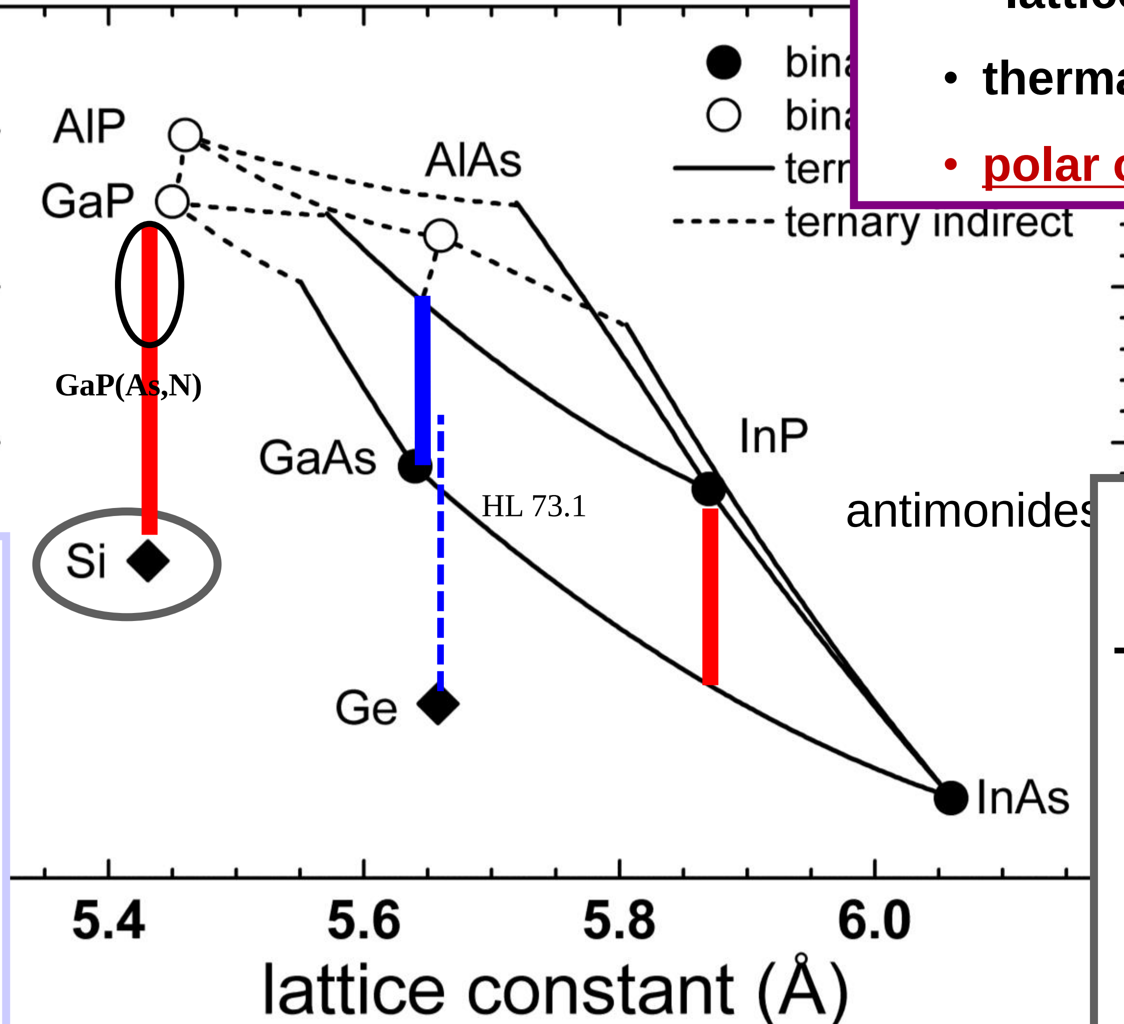




O. Supplie, …
T. Hannappel
Phys. Rev. B,
in print
….

S. Brückner, …, T. Hannappel
New J. Phys. 15 (2013) 113049
O. Supplie, T. Hannappel, …
Phys. Rev. B 86 (2012) 035308
S. Brückner, …, T. Hannappel
Phys. Rev. B 86 (2012) 195310
….

III-V semiconductor heteroepitaxy on Si(100): potentials and issues



III-V on Si(100)

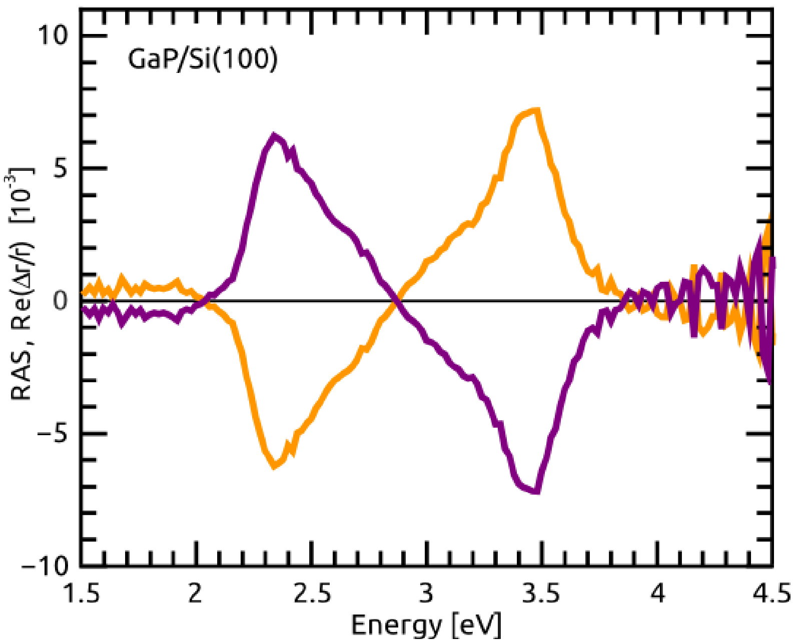
Epitaxial challenges:

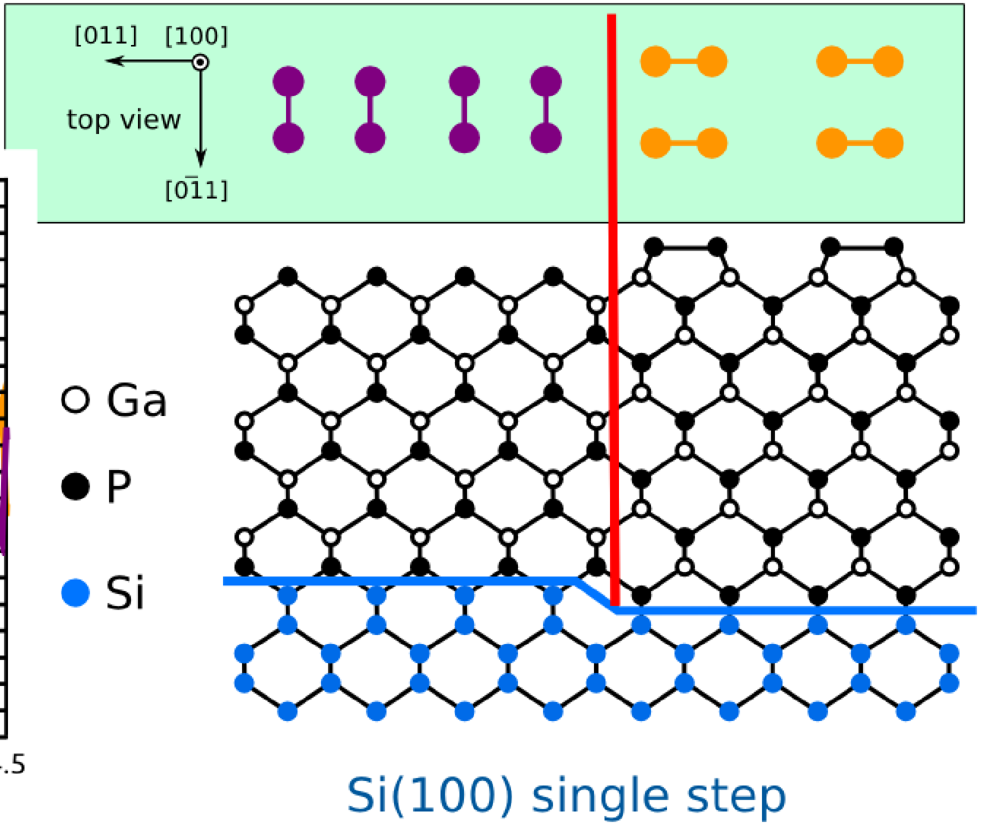
- **lattice constants**
- **thermal expansion**
- **polar on non-polar**

HL 73.1

HL 83.6

In situ RAS: GaP/Si(100)



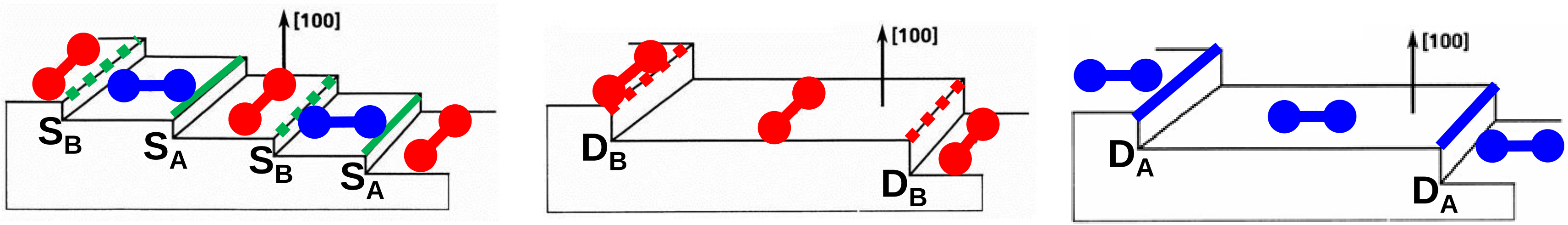


Döscher et al., *Appl. Phys. Lett.* **93** : 172110, 2008.
Kroemer, *J. Cryst. Growth* **87** : 193, 1981.

Hahn, Schmidt et al., *Phys. Rev. B* **68** : 033311, 2003.
Töben et al., *Surf. Sci.* **494** : 755, 2001.

Si(100): Influence of step type and domain ratio on RAS signal

Si(100): (2x1)/(1x2) — Si(100): (2x1) — Si(100): (1x2)

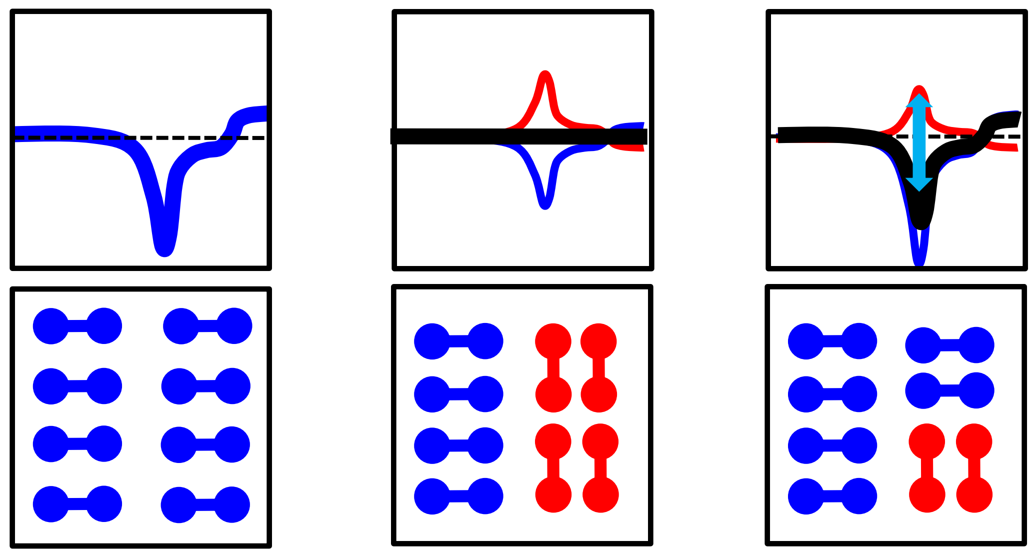


D.J. Chadi, Phys. Rev. Lett. 59 (1987) 1691

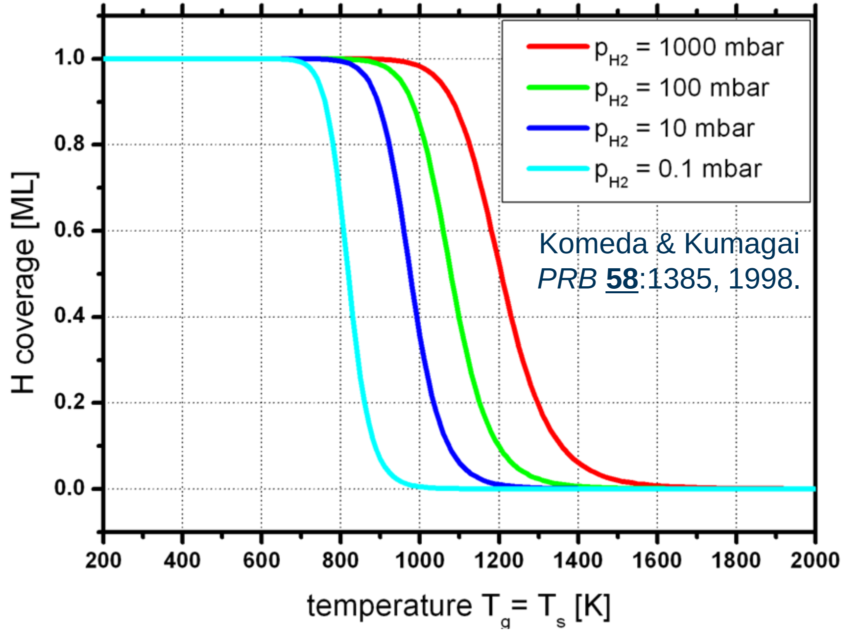
RAS at Si(100):H

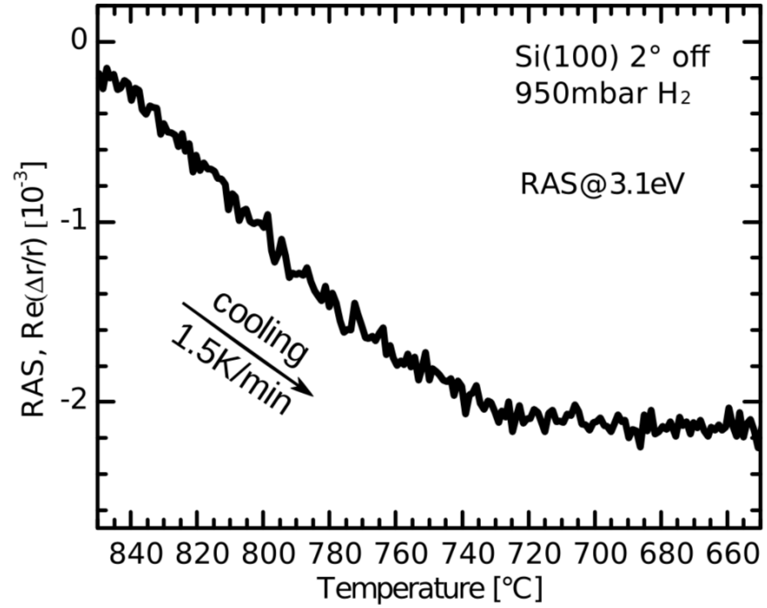
$$\frac{\Delta r}{r} = 2\,\frac{r_{[0\bar{1}1]} - r_{[011]}}{r_{[0\bar{1}1]} + r_{[011]}}$$

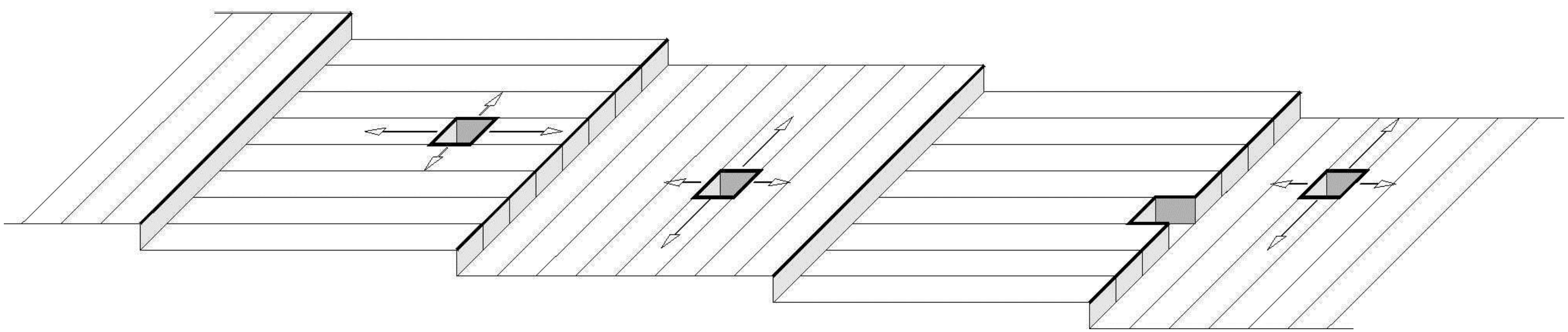
single domain (1x2) — two domain (2x1)/(1x2) — “unequal” domain ratio



Si(100) in H-ambient: D_A steps







vacancy generation + anisotropic diffusion + annihilation at S_B edges

Swartzentruber et al., *Surf. Sci.* **329** : 83, 1995 ; Bedrossian and Klitsner,, Phys. Rev. Lett. **68** : 646, 1992.

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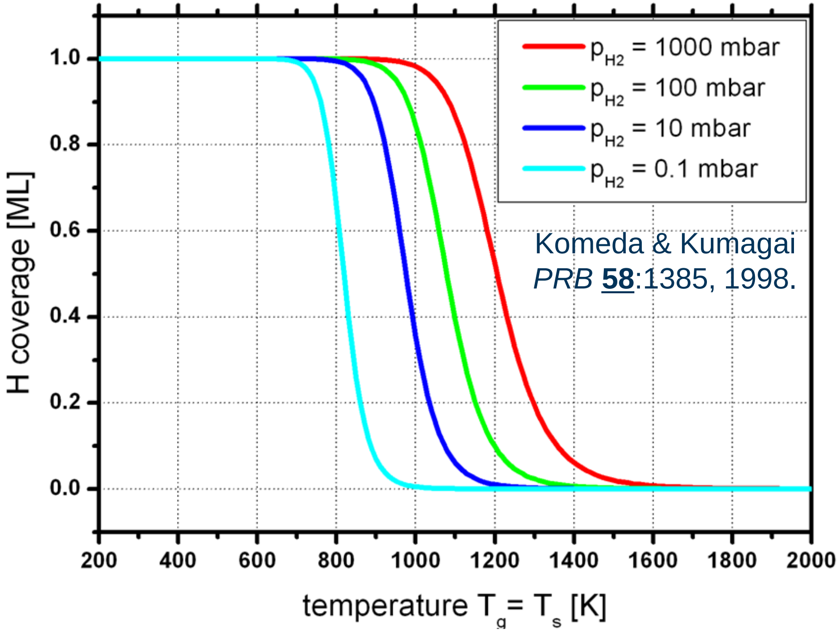

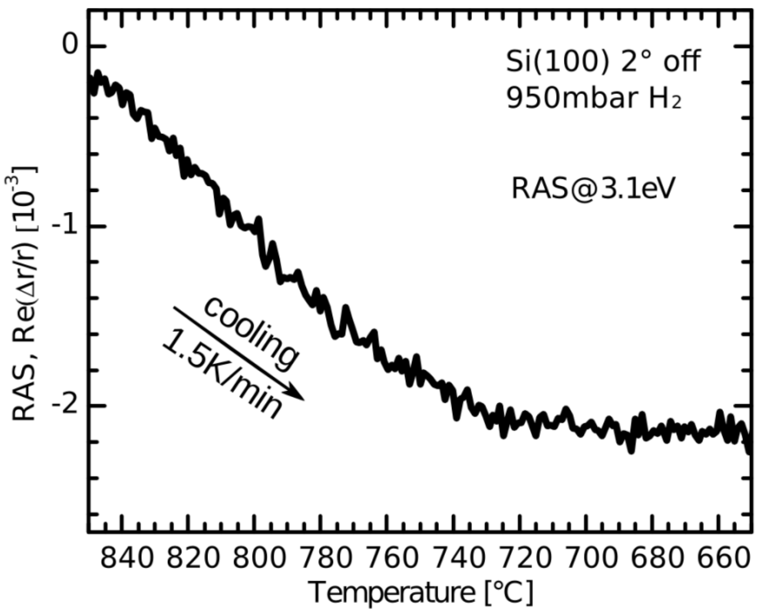

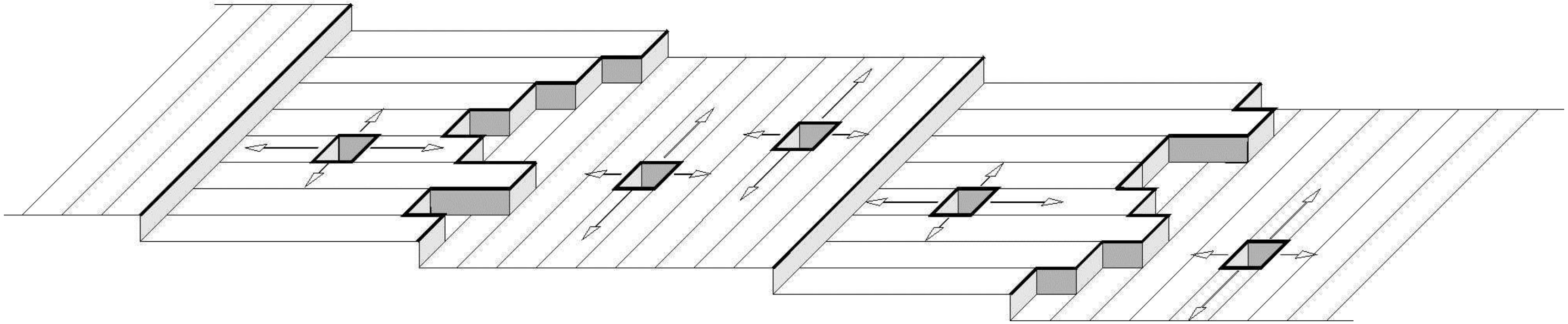

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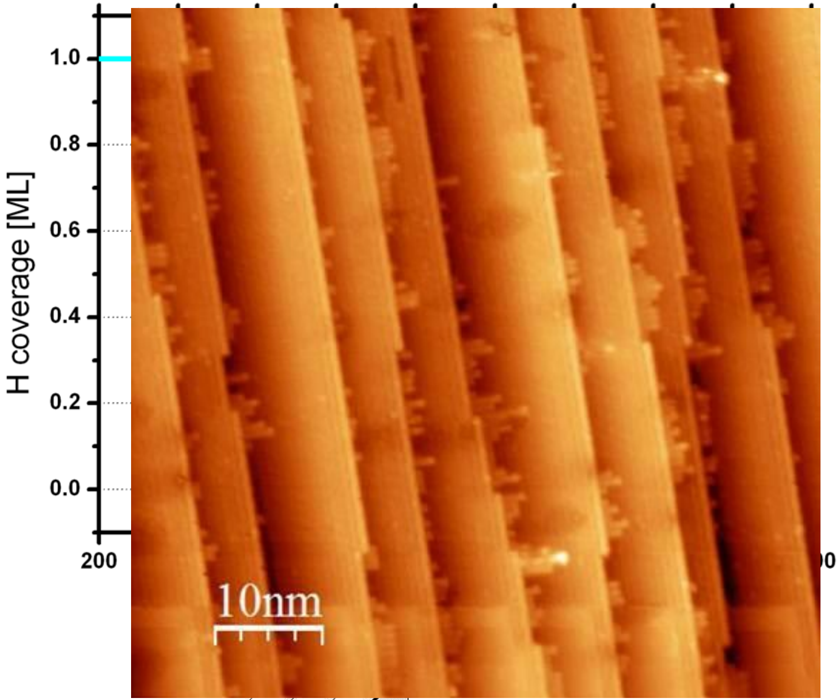

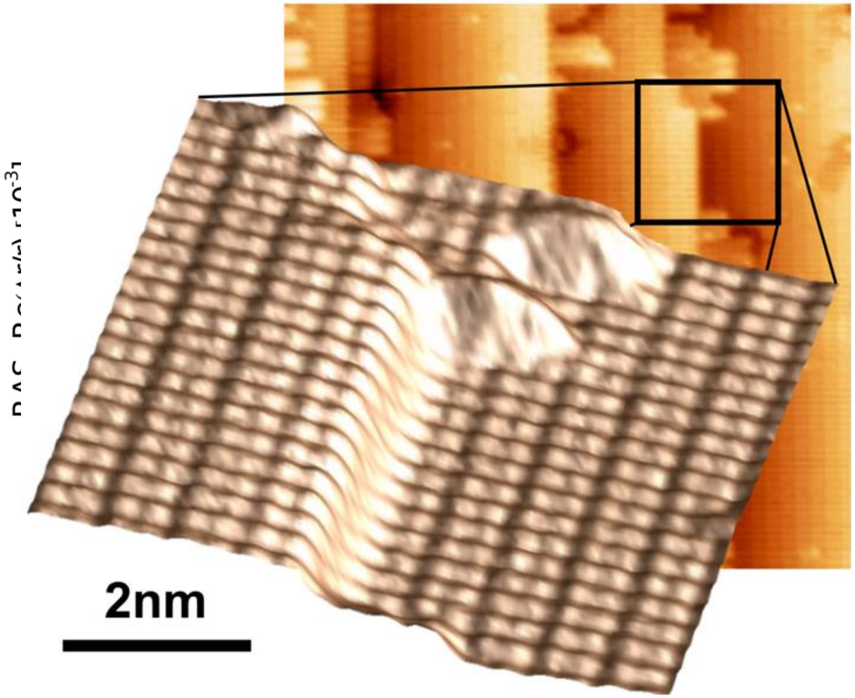

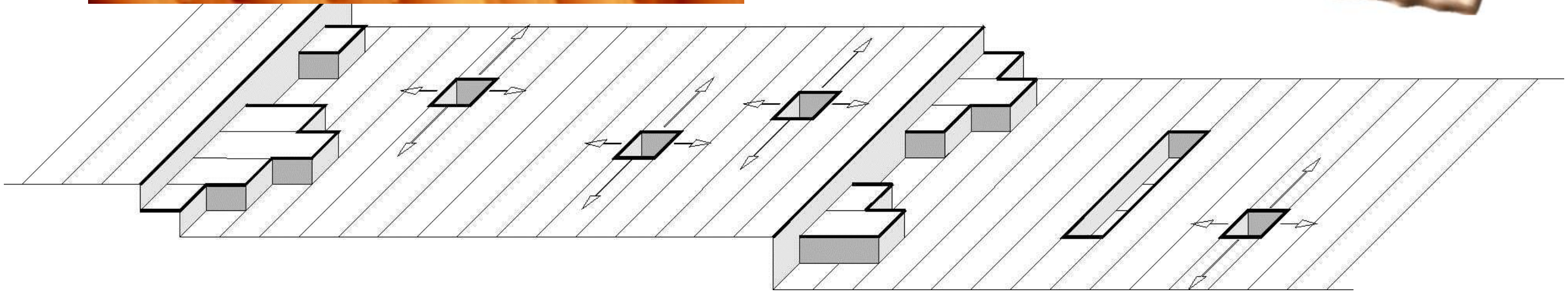

vacancy generation + anisotropic diffusion + annihilation at S_B edges

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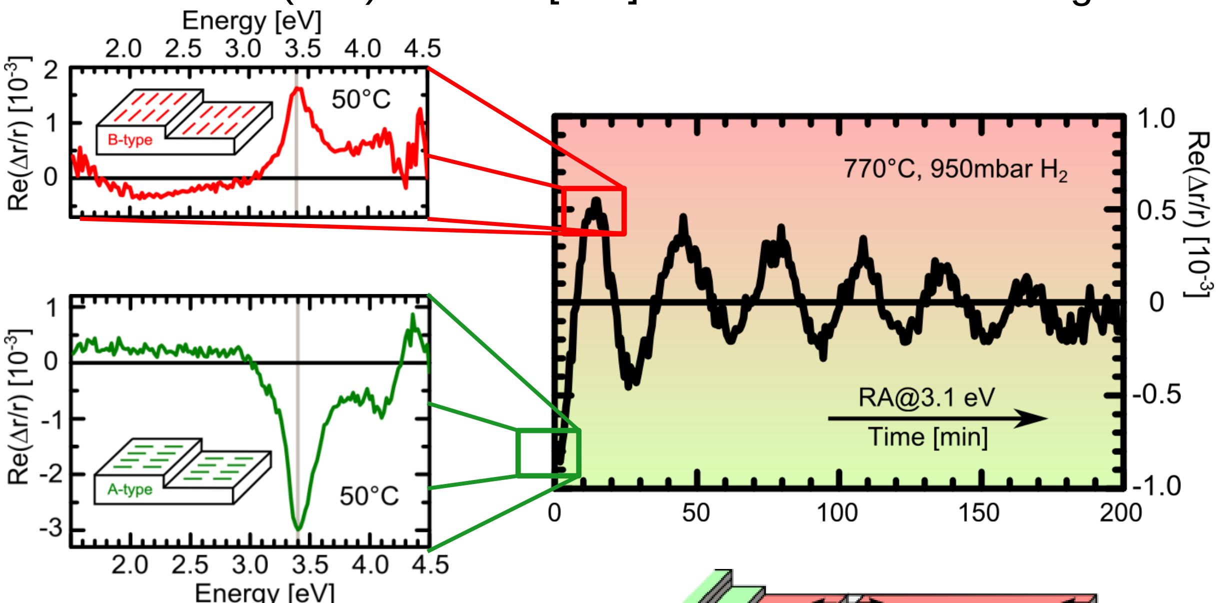
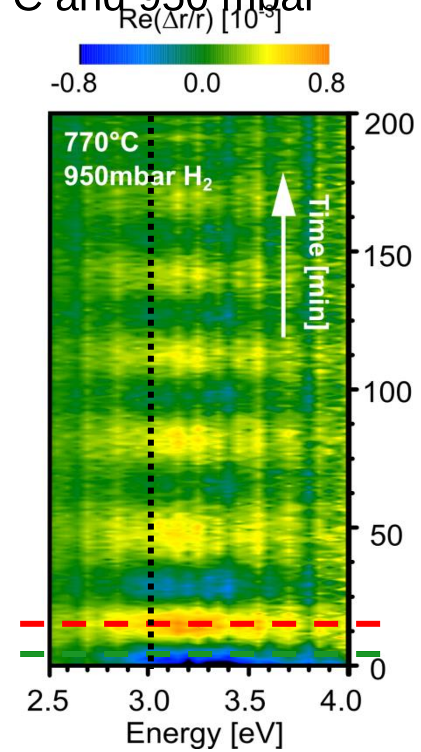
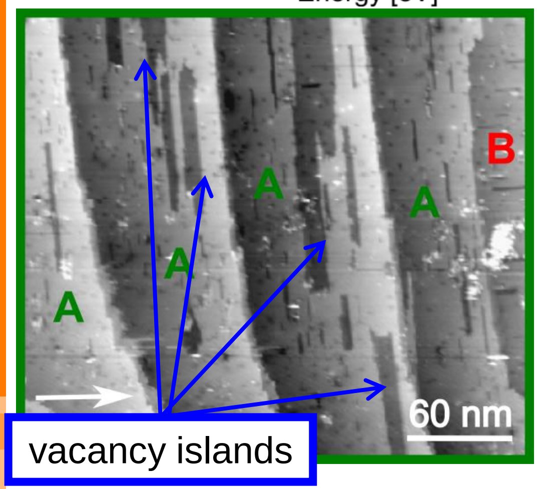
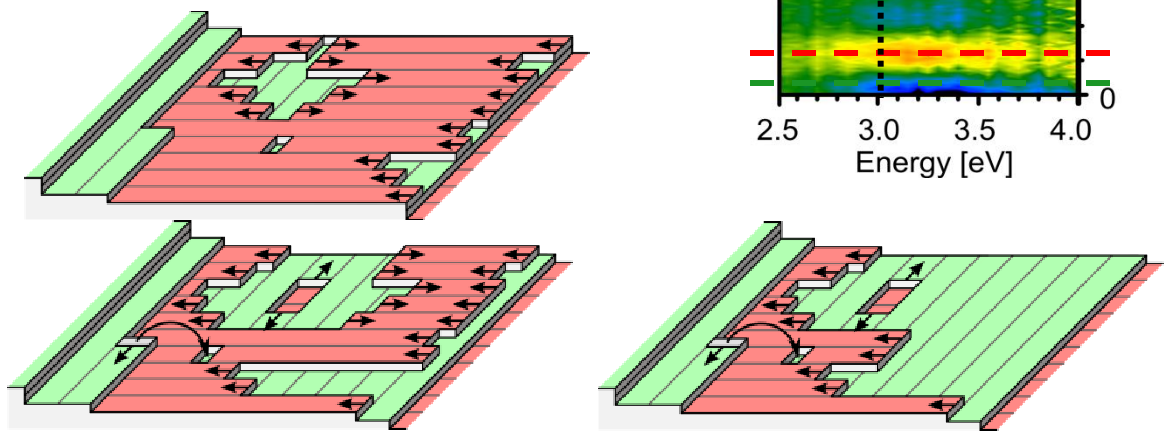
Observation of layer-by-layer removal

In situ RAS at Si(100) 0.1° → [011]: annealing at 770° C and 950 mbar









layer-by-layer removal

S. Brückner et al., **New J. Phys. 15** 113049 (2013)

Brückner, …, Hannappel *Phys. Rev. B* **68** : 195310, 2012.
Brückner, …., Hannappel, New J. Phys. **15** 113049 (2013)

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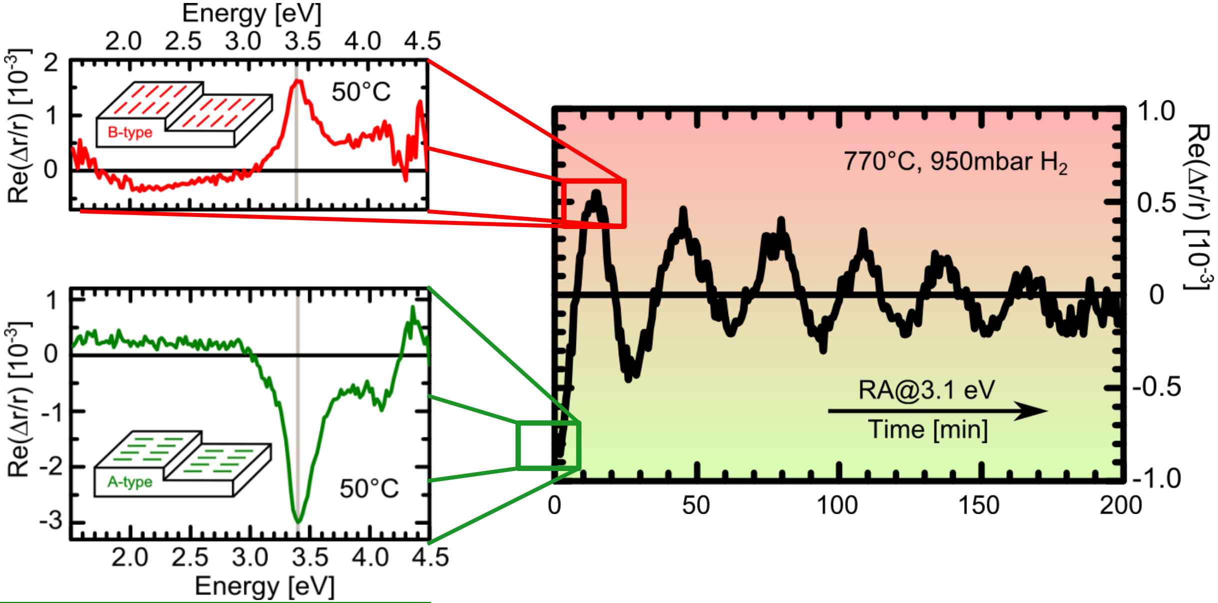
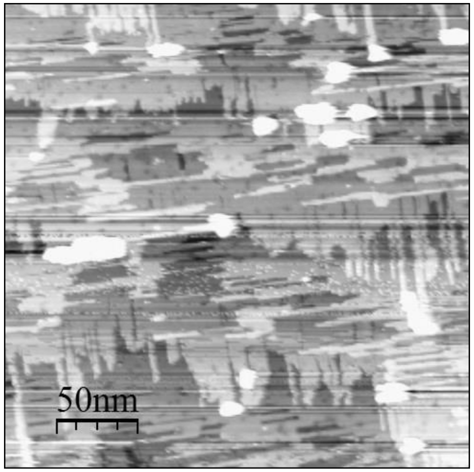
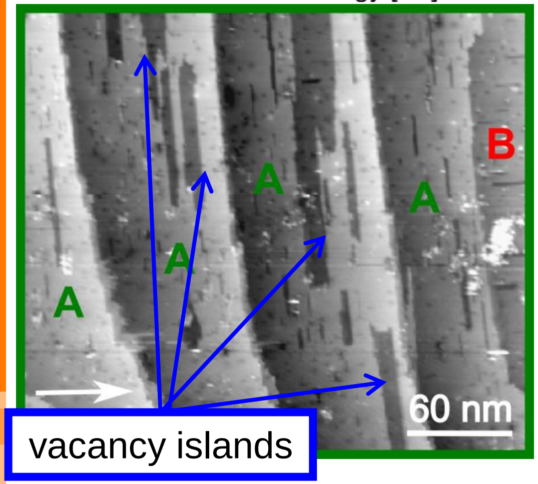






Oscillation = alternating formation of A- and B-type majority domains

- STM → nucleation of vacancies
- anisotropic diffusion of vacancies alongside dimer rows → elongated vacancy islands
- removal of subjacent Si layer limited by size of vacancy island

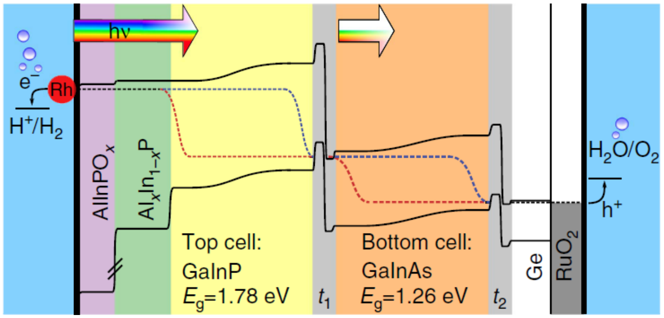
➡ layer-by-layer removal

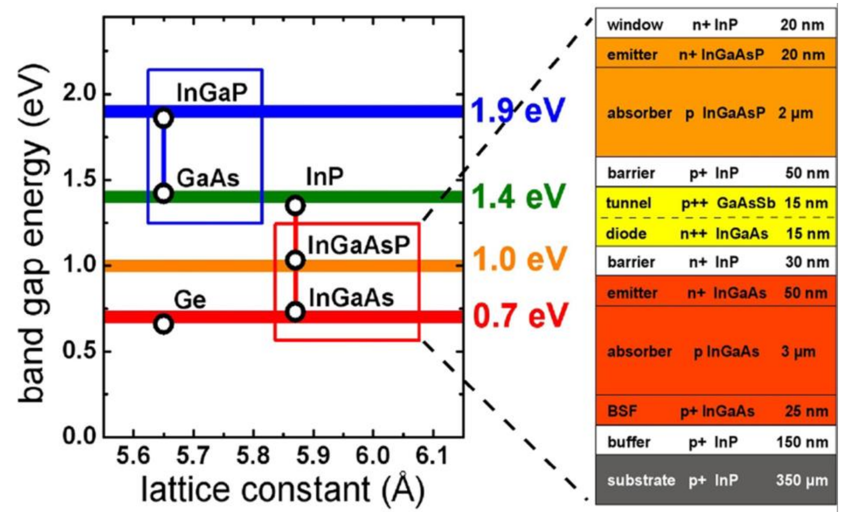
Brückner, …, Hannappel *Phys. Rev. B* **68** : 195310, 2012.
Brückner, …., Hannappel, New J. Phys. **15** 113049 (2013)

Thomas Hannappel

DPG

Conclusion



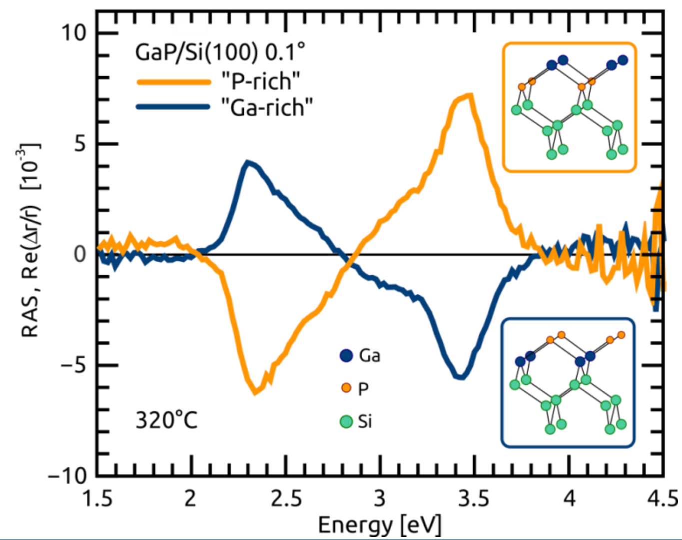


1. Record cell development:

- 46 % in PV, > 50 % accessible
- 14 % in direct solar H-generation,
  » stability, efficiency, catalysis, costs to be addressed

2. III-V on silicon (100)

- atomically abrupt interface
- P-Si bonds at interface



TU Ilmenau: Oliver Supplie, Matthias May, Peter Kleinschmidt, Sebastian Brückner, Christian Koppka, Henning Döscher, Weihong Zhao, Agnieszka Paszuk, Matthias Steidl, Antonio Müller, Philipp Sippel

Uni Duisburg-Essen: Werner Prost, F-J. Tegude

Helmholtz-Zentrum Berlin: Roel van de Krol, Rainer Eichberger, Klaus Schwarzburg, Christian Höhn

Paul Drude Institut: Frank Grosse, Alexandre Romanyuk

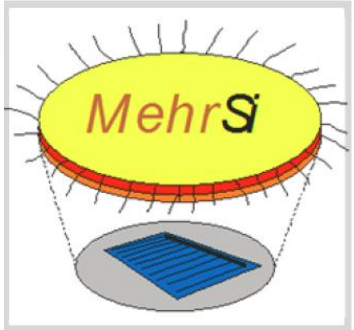
Fraunhofer ISE: Frank Dimroth, Andreas Bett

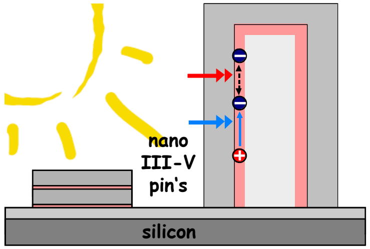
Azur Space: Thomas Bergunde, Kristof Möller

CalTech: Achim Lewerenz, Harry Atwater

Aixtron SE: Michael Heuken

Bundesministerium für Bildung und Forschung





DFG
(HA3096/4-1)

Thank you!