Semiconductor Nanomaterials in Renewable Energy Applications

Bohdana NAIDYCH

Vasyl Stefanyk Precarpathian National University

Physical-Technical Faculty

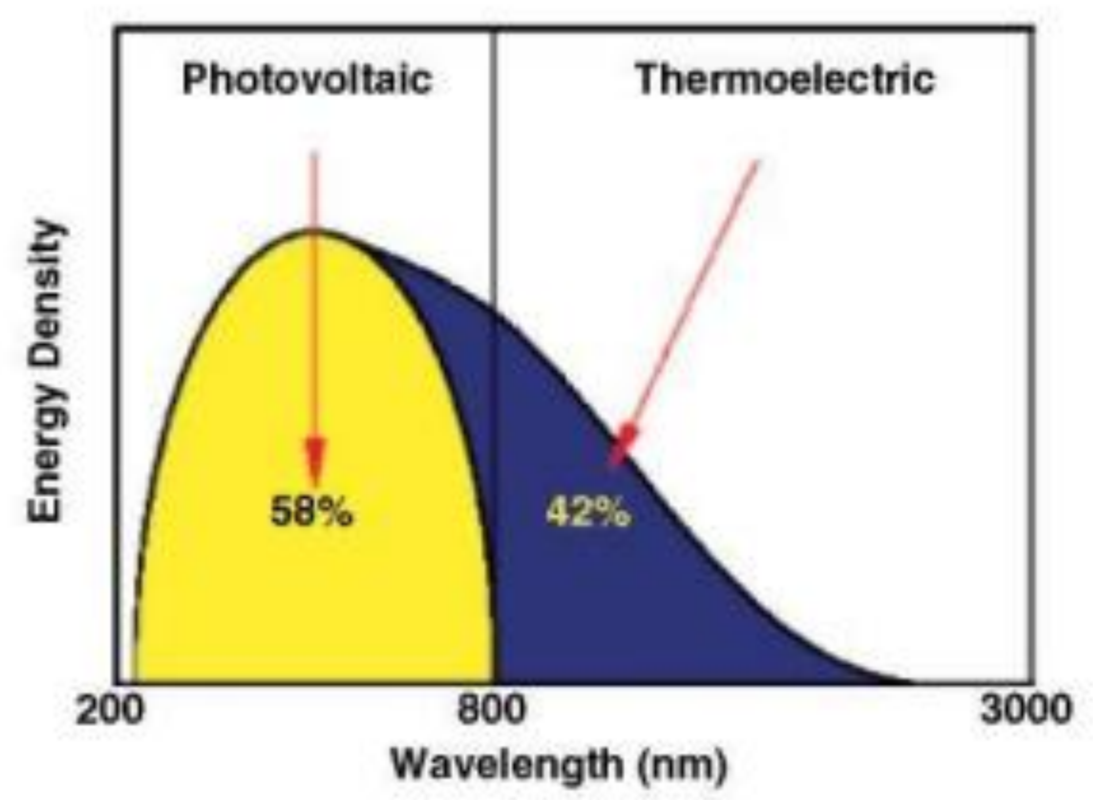
Department of Physics and Chemistry of Solids

Supported by EIT Manufacturing

Funded by the European Union

EIT HEI Initiative — Innovation Capacity Building for Higher Education — eit-hei.eu

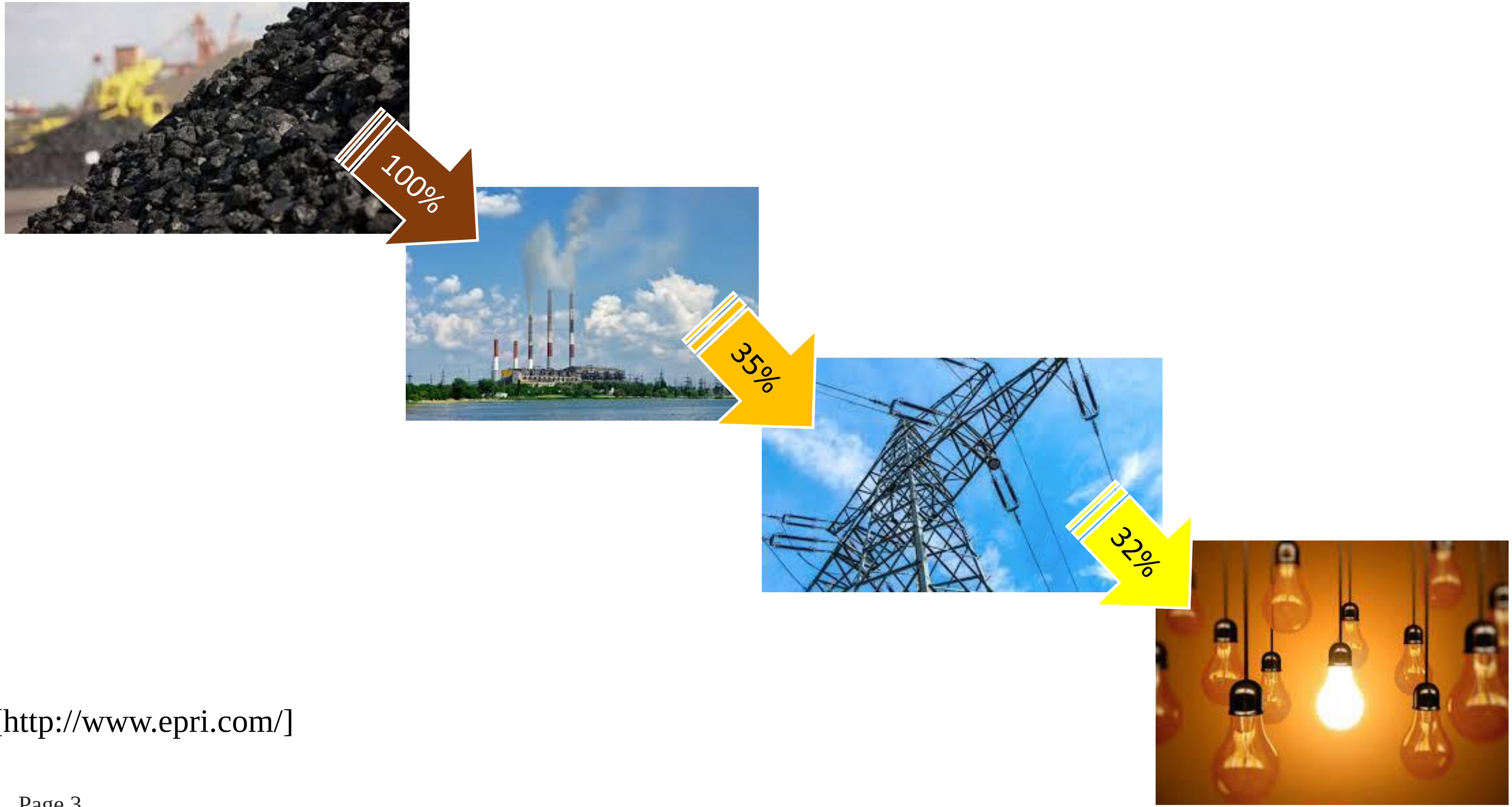
Sun – the Greatest Source of Energy



Simplified solar spectrum and energy ratios to be used within the PV cell and the TEG

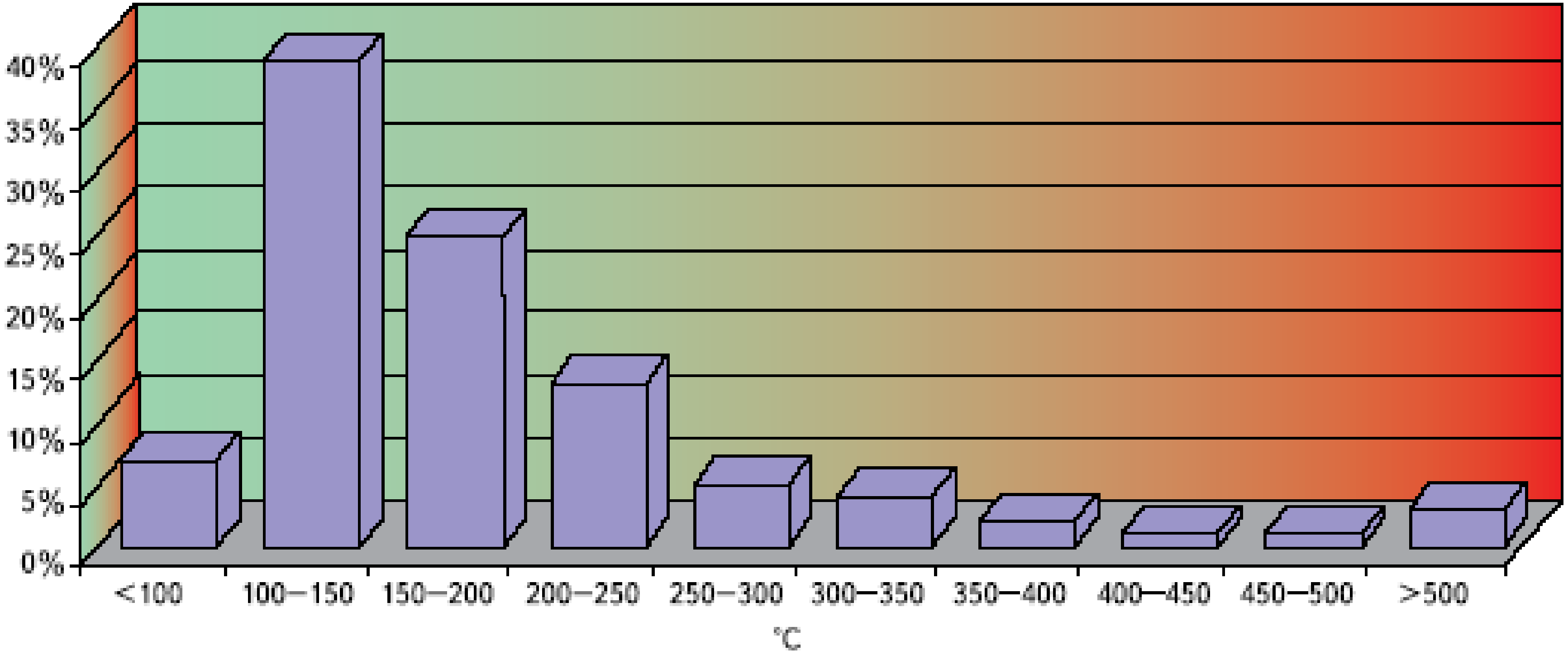
[Elsarrag E. et al., Spectrum splitting for efficient utilization of solar radiation: a novel photovoltaic–thermoelectric power generation system. Elsarrag et al. Renewables (2015) 2:16]

Why thermoelectrics and photovoltaics?



[http://www.epri.com/]

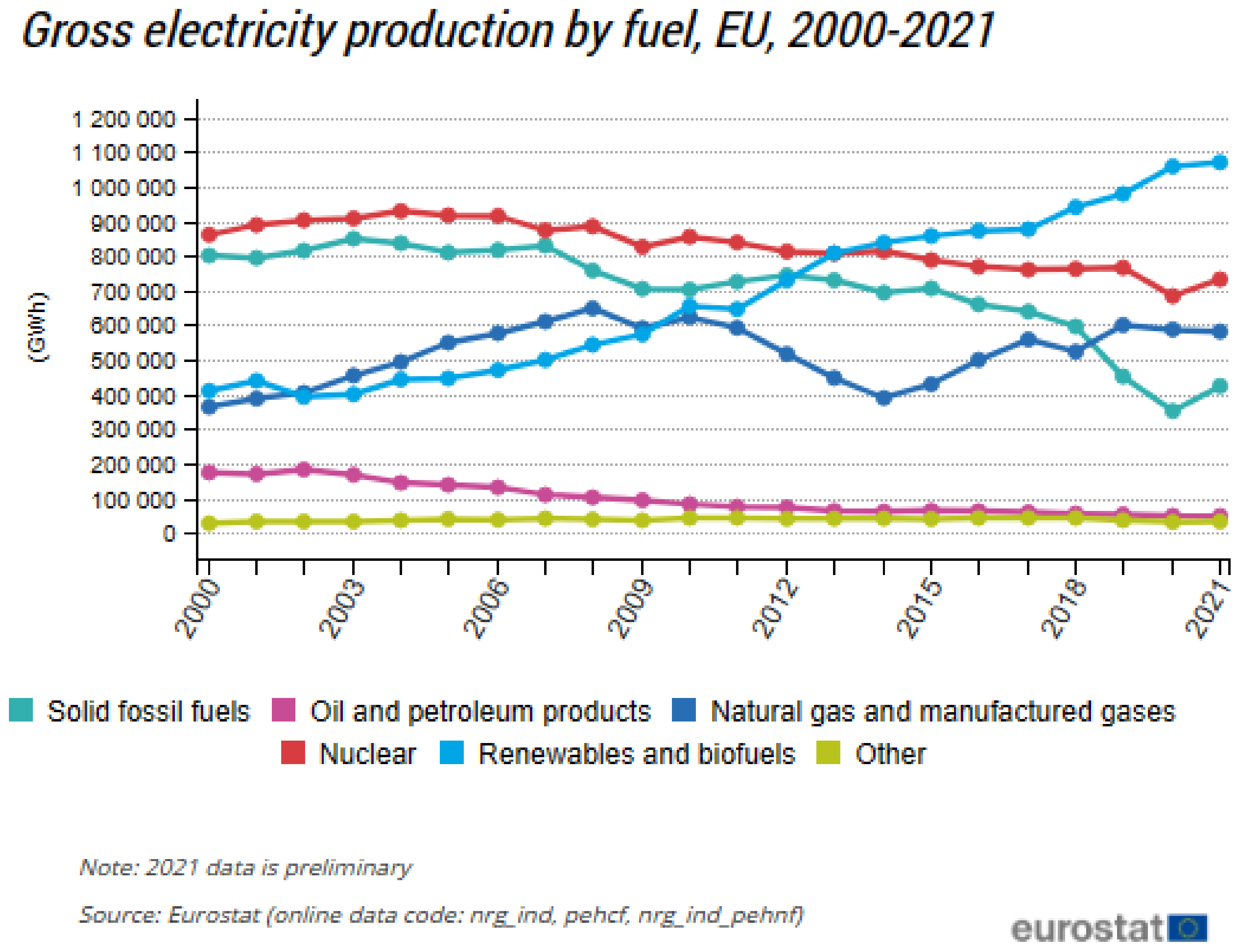
The loss of heat in the environment

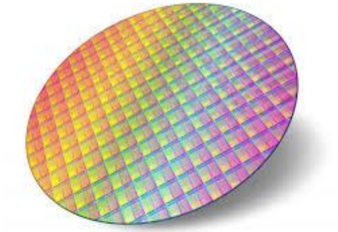


Temperature distribution on the surface of industrial units

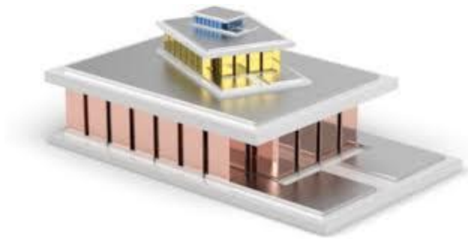
[P. Shestakovsky. Thermoelectric alternative sources. New technologies. No 12. 131 (2010).]

Why thermoelectrics and photovoltaics?





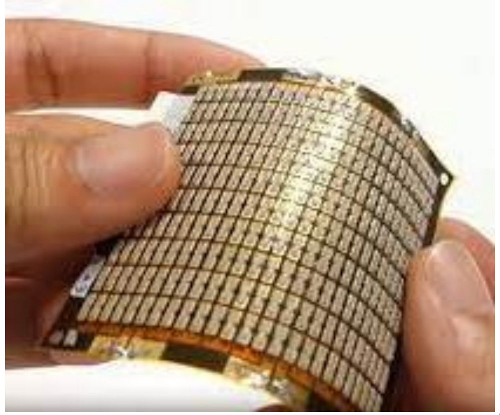
Why thermoelectrics and photovoltaics?



REGINNA 4.0

- Clean and pollution-free
- Low operating costs
- High reliability and no moving components
- Maintenance-free operation without noise
- The price of solar panels is currently decreasing
- Small and easily integrated into an existing setup
- Energy is converted directly (no intermediate energy conversion)
- Wide range of power generation from kW to μW

Content



1. Development of thermoelectricity and photovoltaics. Transition to nanoscale elements
2. Methods of obtaining semiconductor nano-size materials
3. Peculiarities of the structure and properties of semiconductor nanomaterials
4. Practical application of nanomaterials
5. Characterization of nanomaterials

1) Select a scenario of interest for you:

electronic devices of a small airplane

kitchen equipment

touristic camping

doctors’ tablet or laptop

sports equipment

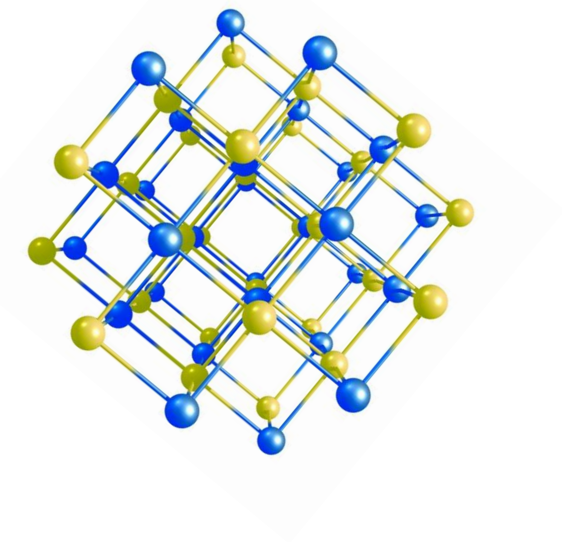
the “most popular” device

2) Where could an additional power source be useful in your chosen scenario?

3) For your report, lookout for answers to:

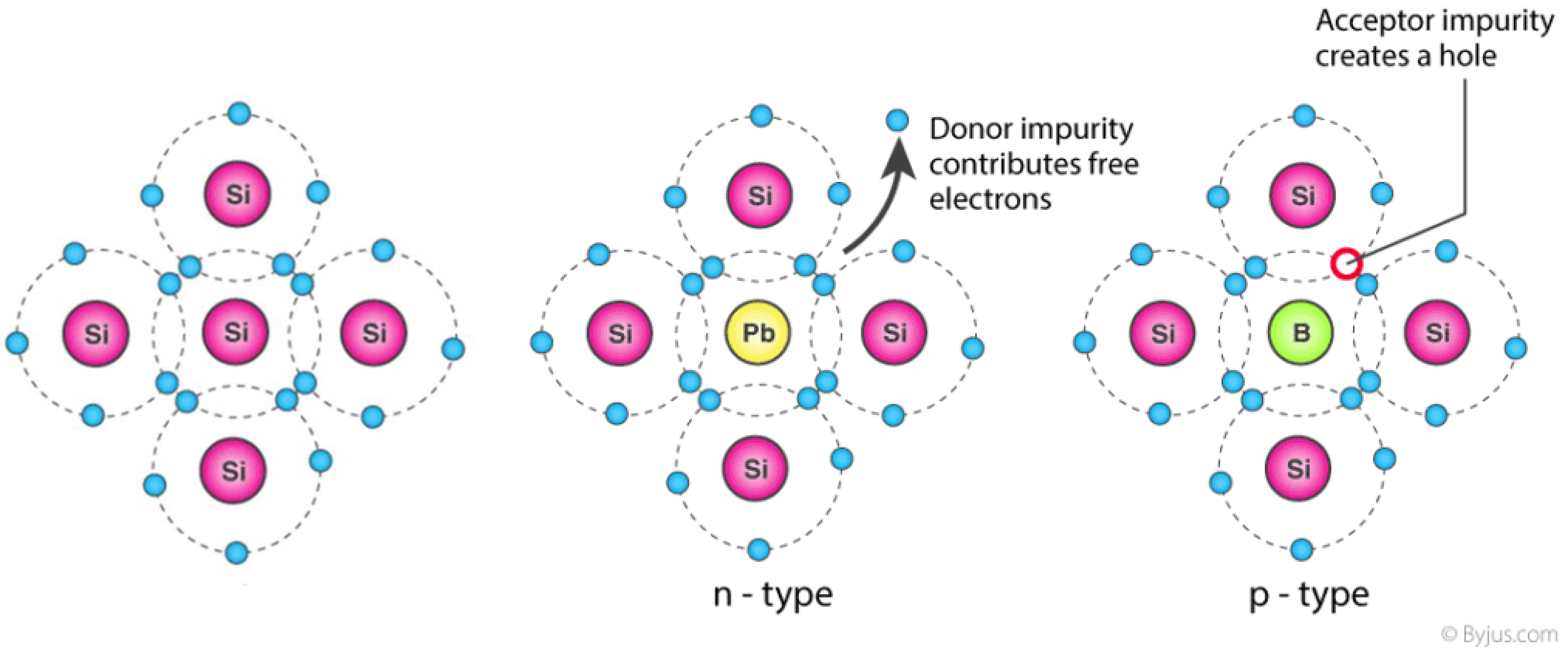
- Prerequisites: Description of needed materials (e.g., chemical formula, space dimensions)
- Production: What equipment do you need to obtain the sample/material needed in the device?
- Measurement and Modeling: How can you check the parameters of the device?
- Details in your chosen scenario: Where should this device be placed?

REGINNA 4.0



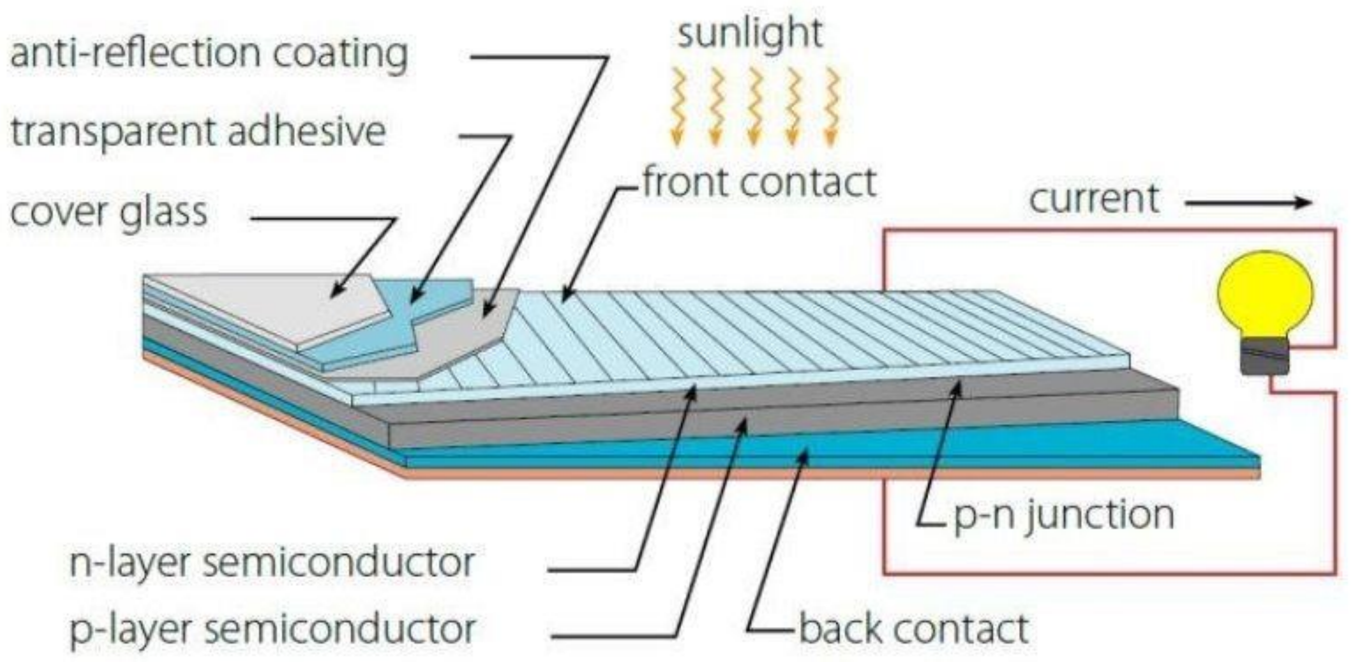
I. Development of thermoelectricity and photovoltaics. Transition to nanoscale elements

Semiconductors



[https://www.rs-online.com/designspark/what-are-semiconductors-definition-types-industries]

Physical principles of photovoltaics



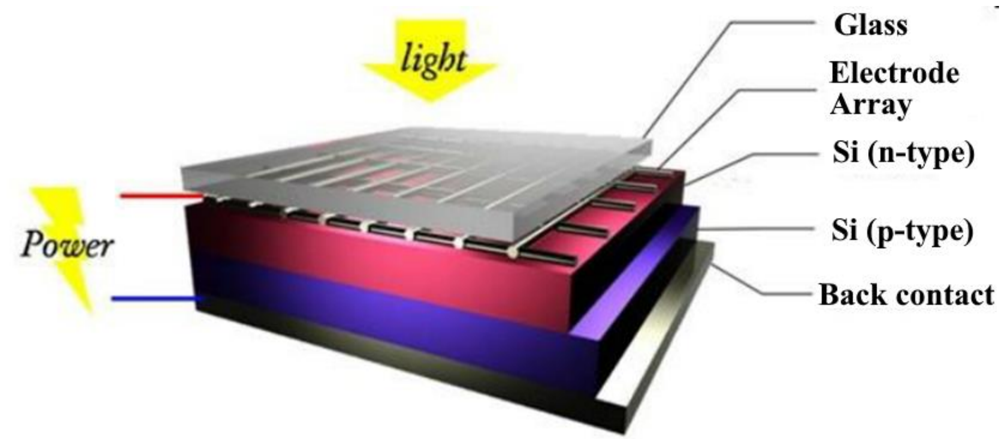
Types of solar modules:

- monocrystalline
- polycrystalline
- thin-film solar module

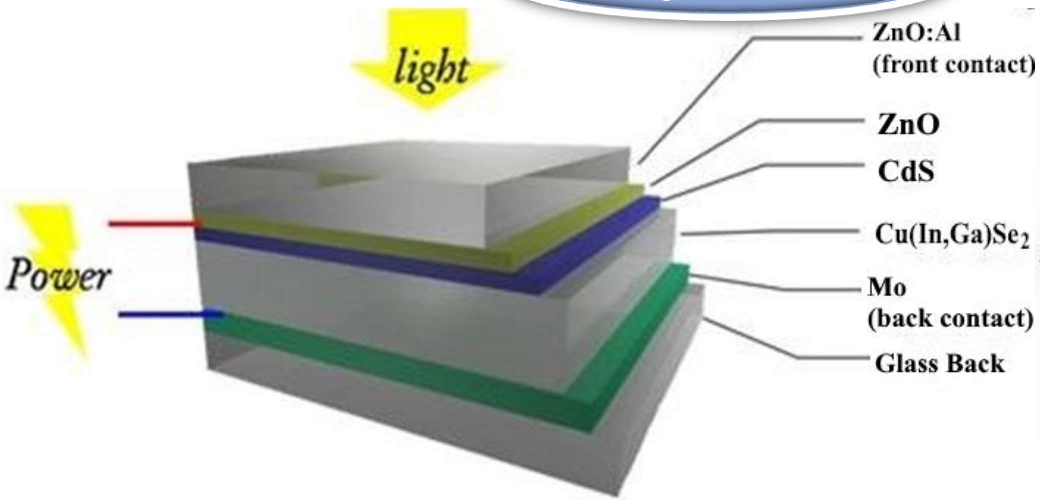
[https://www.insightsonindia.com/2022/08/10/indias-solar-power-dream/]

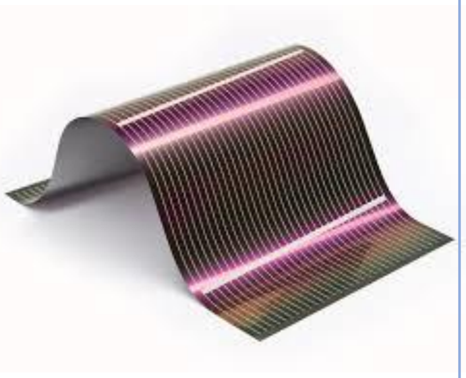
Development of photovoltaic devices

1st generation

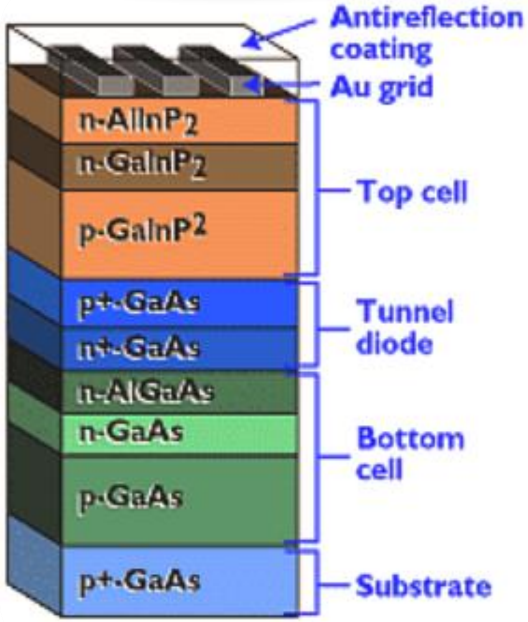


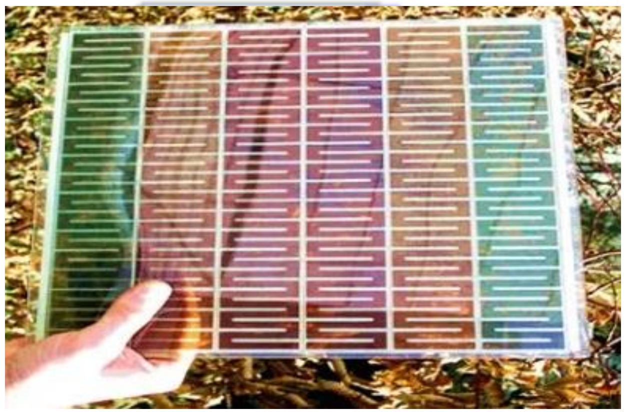
2nd generation





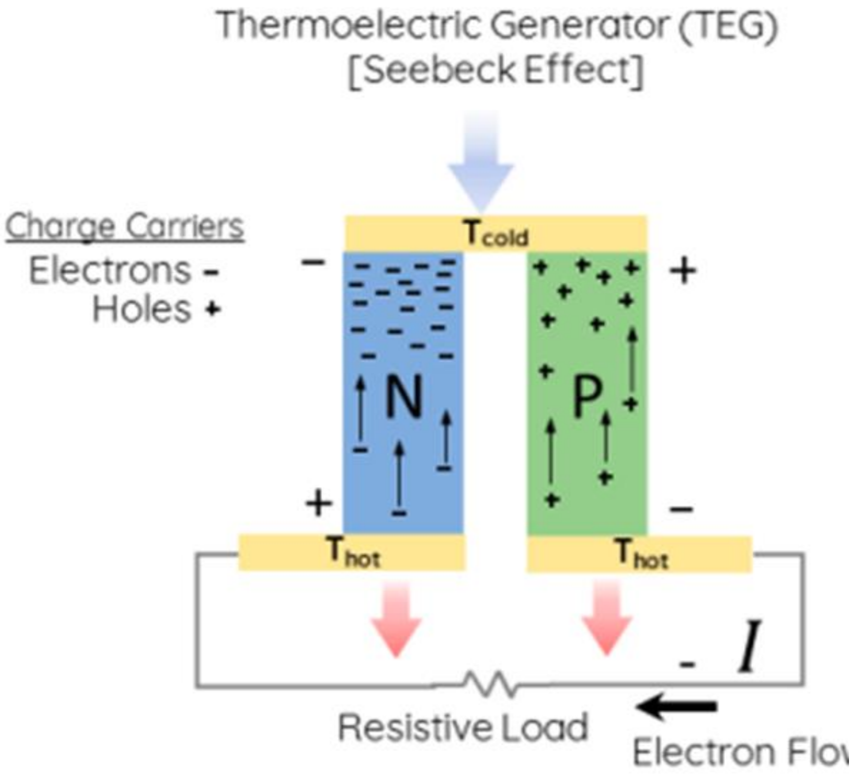
3rd generation



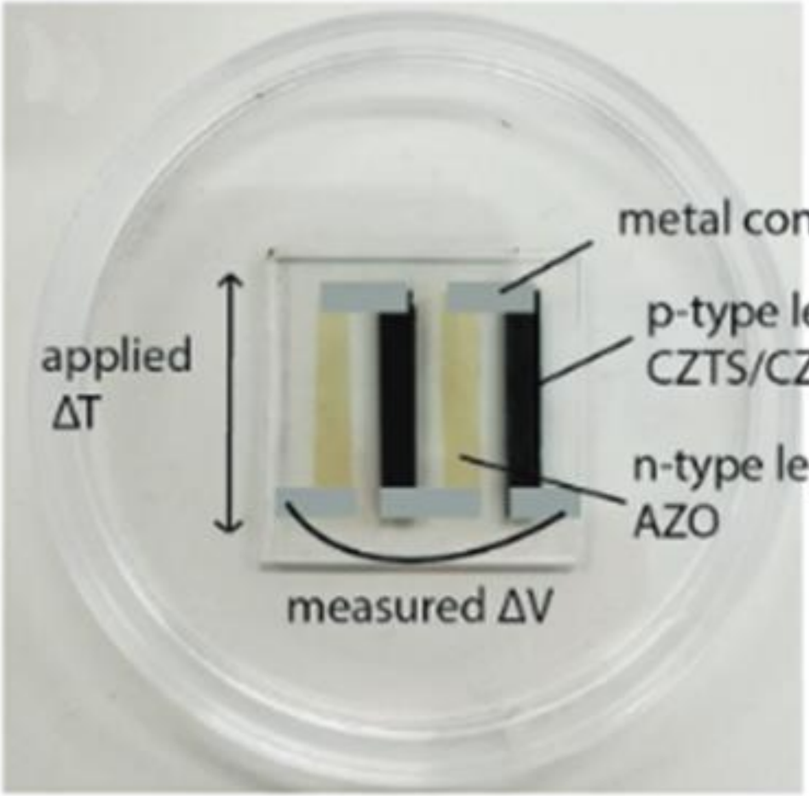


[https://www.ncbi.nlm.nih.gov/pmc/articles/PMC5917436/]

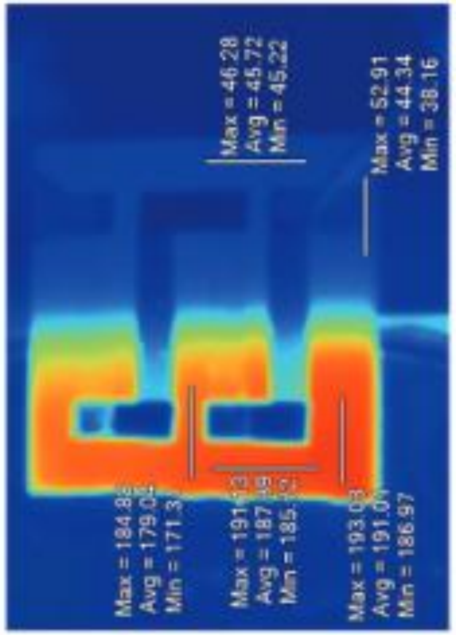
Physical principle of thermoelectric devices



Charge carriers diffuse away from the hot end. Buildup of charge at the cold end produces a voltage potential



Picture of the realized devices for both $Cu_{2.125}Zn_{0.875}SnS_4$ (CZTS) and $Cu_{2.125}Zn_{0.875}SnSe_4$ (CZTSe) p-side and in standard (2 p–n couples) configuration.



Thermography of the TEG device under operation

[Isotta E., et. al. (2022). Advanced Functional Materials, 32(32), 2202157.]

Physical principles of thermoelectric power generation

The figure of merit ZT is defined as

$$ZT=(S^2\sigma)T/\kappa$$

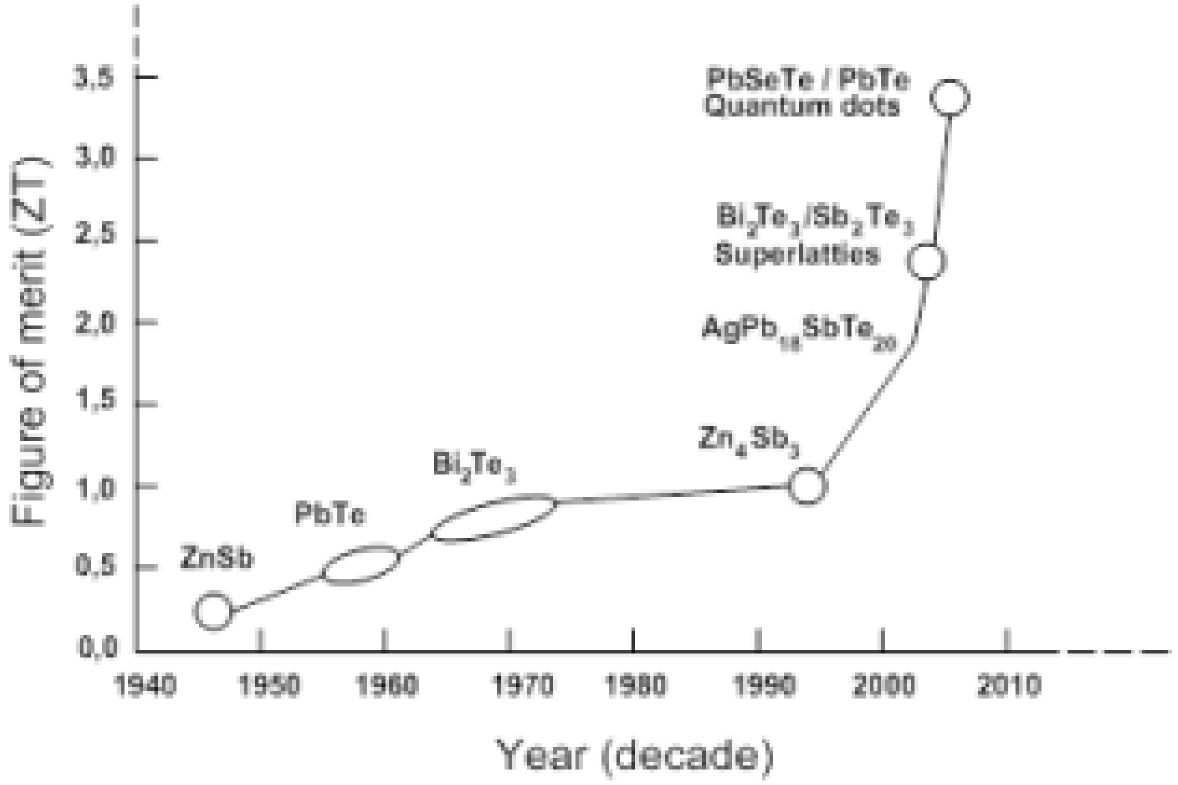
where $(S^2\sigma)$ is a power factor,

S - Seebeck coefficient,

σ - electrical conductivity,

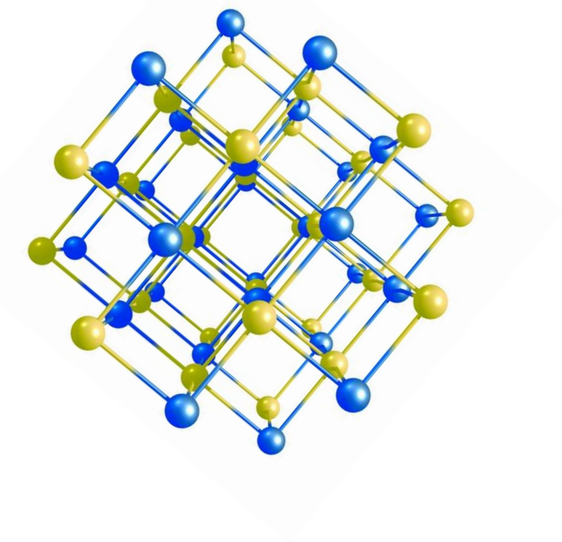
T - absolute temperature, and

κ - thermal conductivity.

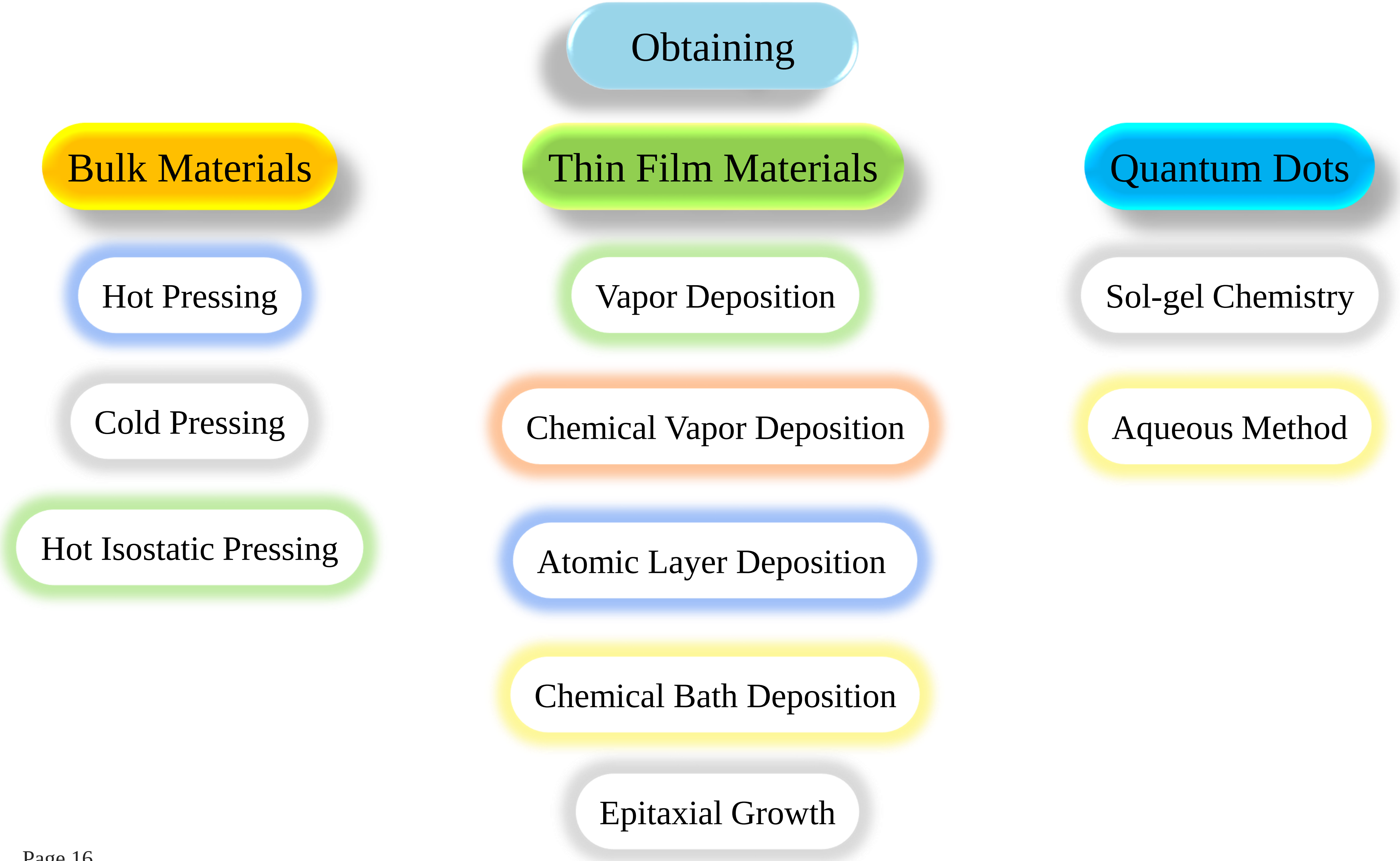


The evolution of the figure of merit (over the years).

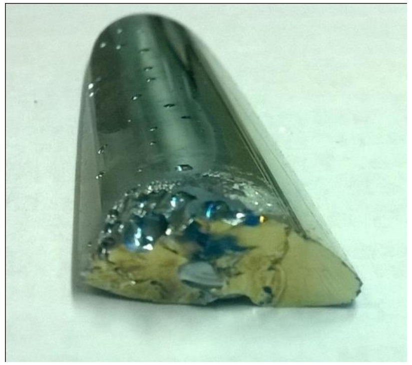
[http://www.sel.eesc.usp.br/jcarmo/pdfs/PUBLICACOES/CAPITULOS/CAP07.pdf]

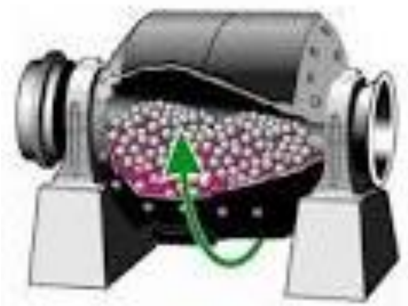


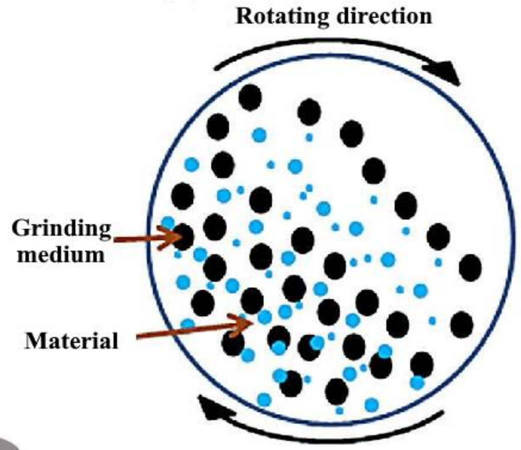
II. Methods of obtaining semiconductor nano-sized materials

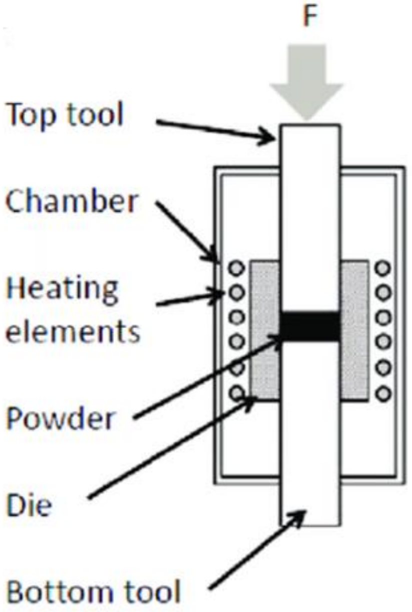

Obtaining
Bulk Materials
Hot Pressing
Cold Pressing
Hot Isostatic Pressing
Thin Film Materials
Vapor Deposition
Chemical Vapor Deposition
Atomic Layer Deposition
Chemical Bath Deposition
Epitaxial Growth
Quantum Dots
Sol-gel Chemistry
Aqueous Method

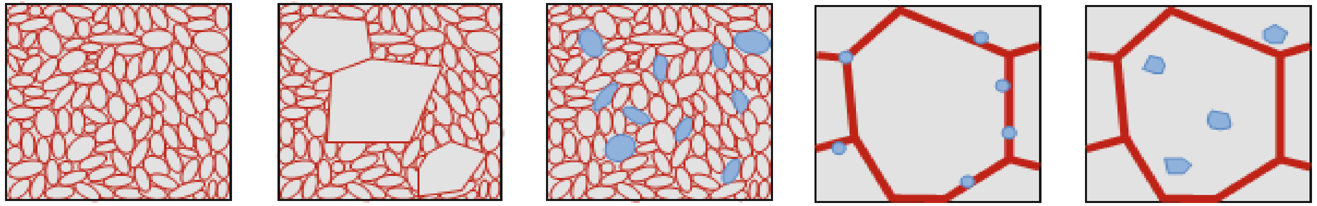
From powder to thermoelectric material

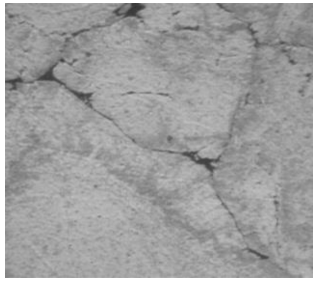






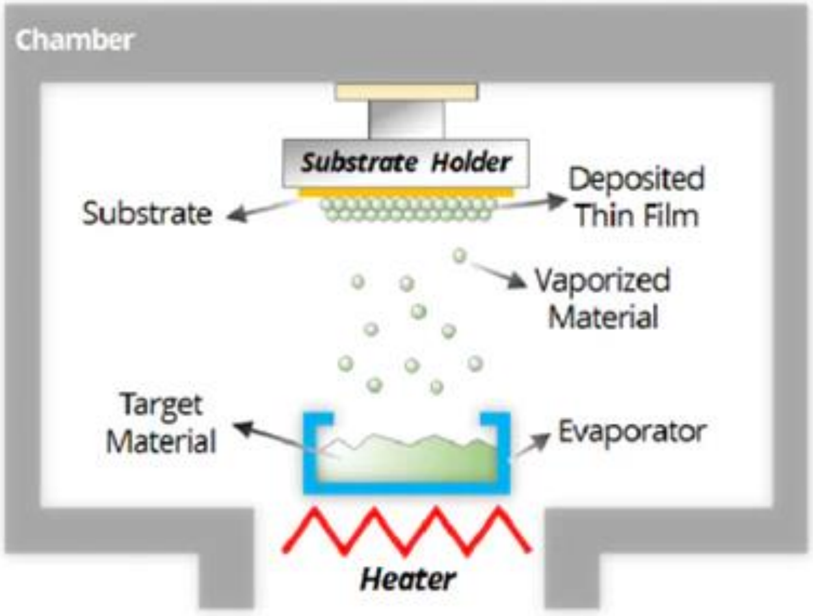






[https://specac.com/product/sample-preparation-equipment/p6-planetary-ball-mill/]

Obtaining of thin films by Vapor Deposition



Scheme of thermal evaporation deposition

(Park et al. 2016)

soda-lime glass (SLG), Al-doped ZnO (AZO); $Cu_{2.125}Zn_{0.875}SnS_4$ (CZTS) and $Cu_{2.125}Zn_{0.875}SnSe_4$ (CZTSe)

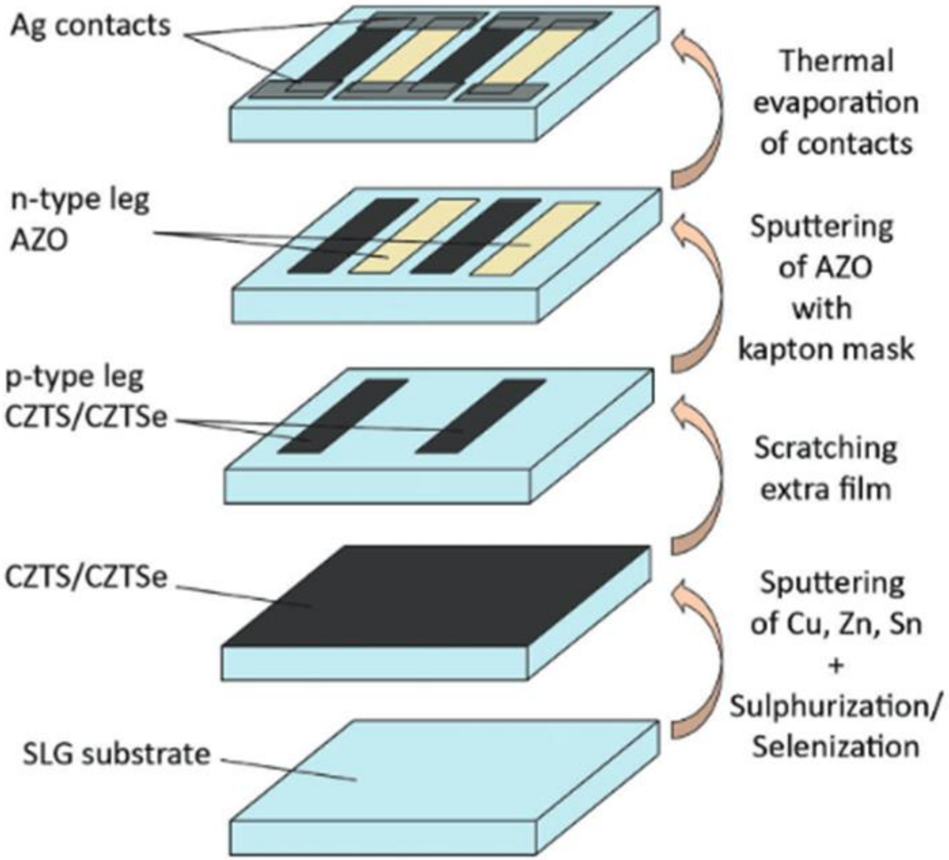
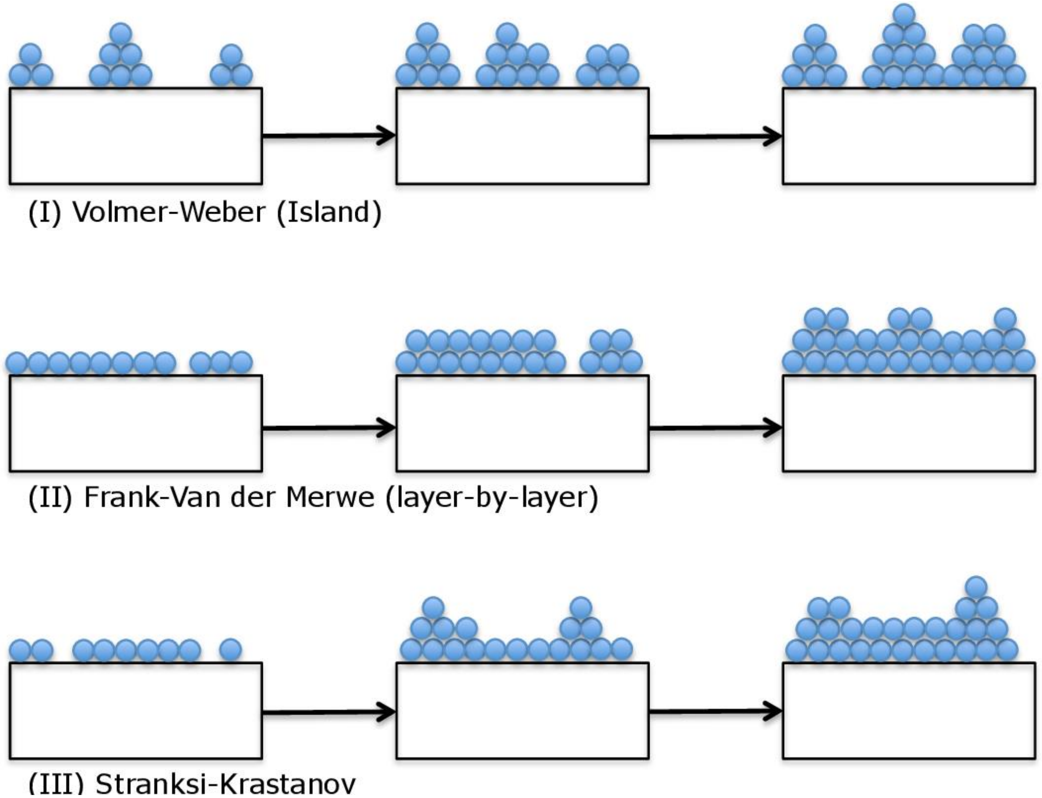


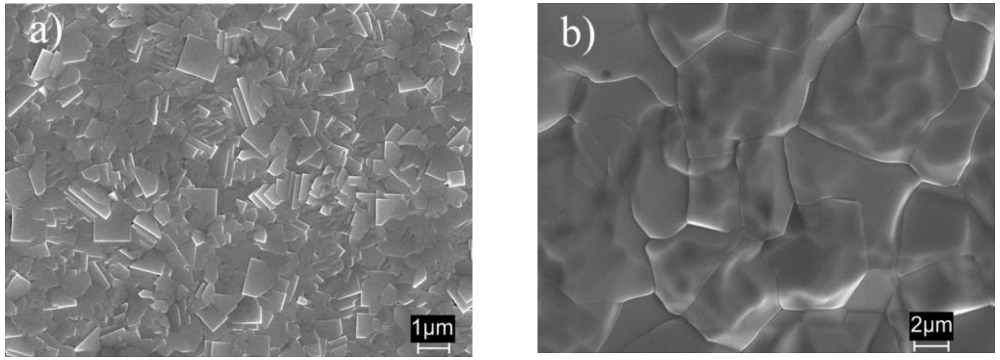
Illustration of the steps of thin film fabrication.

[Izotta E, et al., Advanced Functional Materials, 32(32), 2202157.]

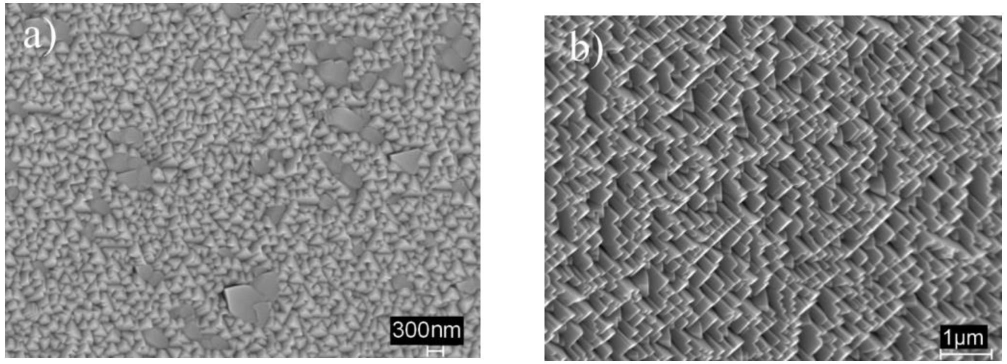
Obtaining of thin films by Vapor Deposition



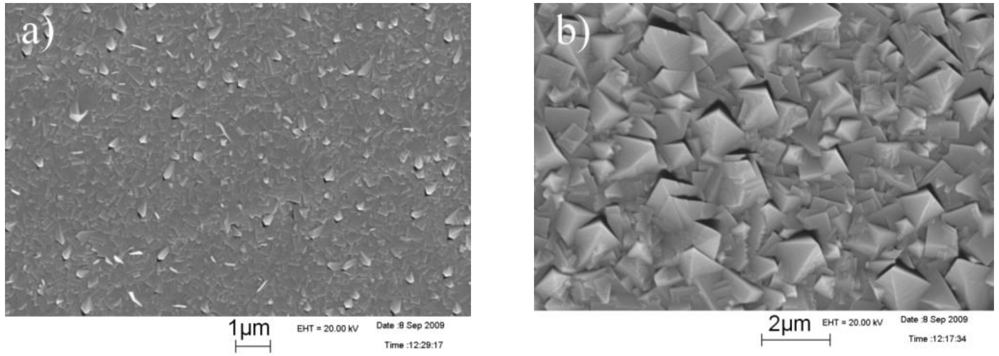
[Powell, Michael. (2015). VO_2 Thin Films and Nanoparticles, from Chemical Vapour Deposition and Hydrothermal Synthesis, for Energy Efficient Applications.]



PbTe / Glass

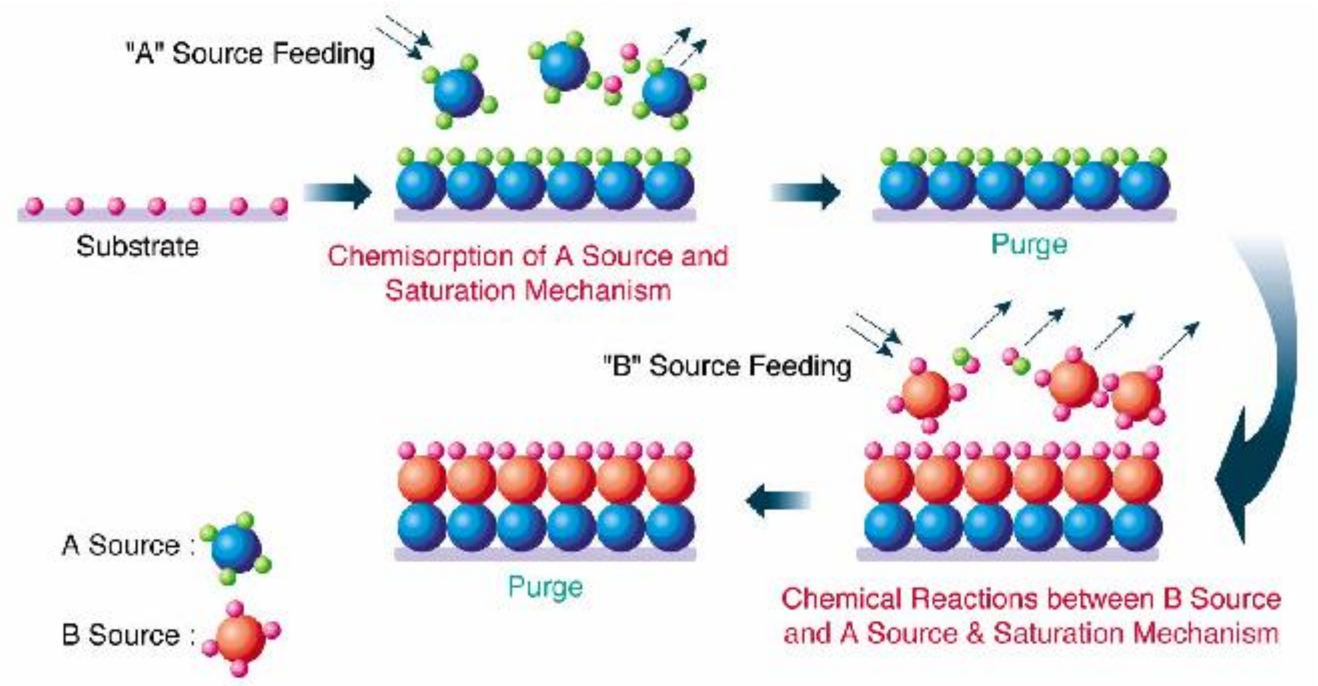


PbTe / Mica



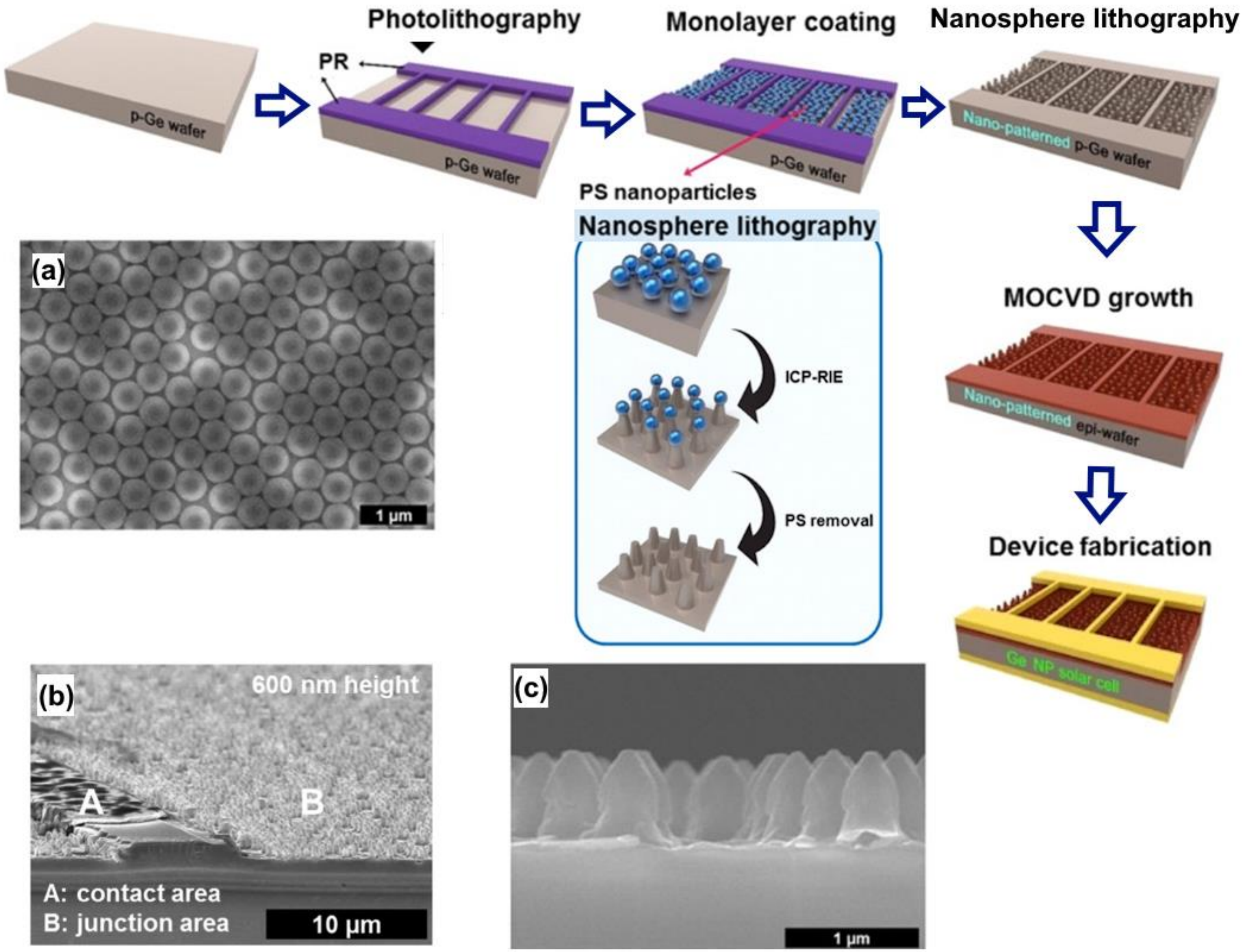
PbTe / SiO_2

Obtaining of thin films by Atomic Layer Deposition



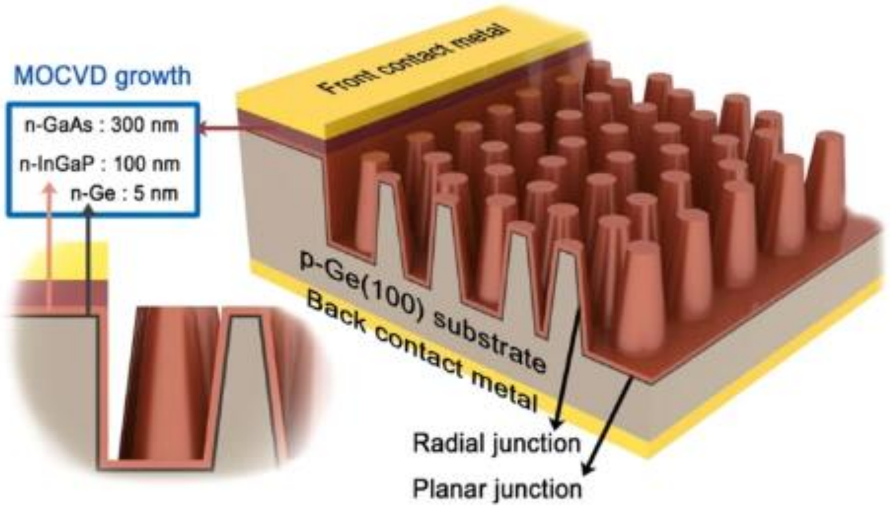
[Hwang C. (2012) ALD(Atomic Layer Deposition) Process Technology in the Semiconductor Industry. Physics and High Technology, 21. p.37]

Obtaining of thin films by Metalorganic Chemical Vapor Deposition

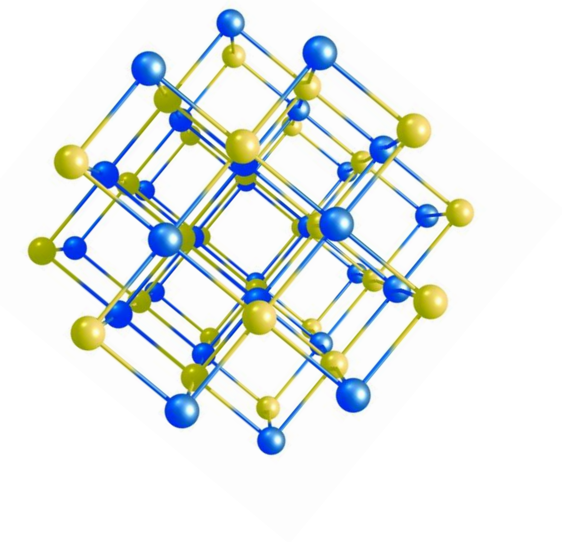


Illustrations of the selective patterning process and cross-sectional SEM images (a, b, c) of the Ge NP solar cells.

[Kim, Y. *et al*. Ge nanopillar solar cells epitaxially grown by metalorganic chemical vapor deposition. *Sci. Rep.* **7**, 42693].

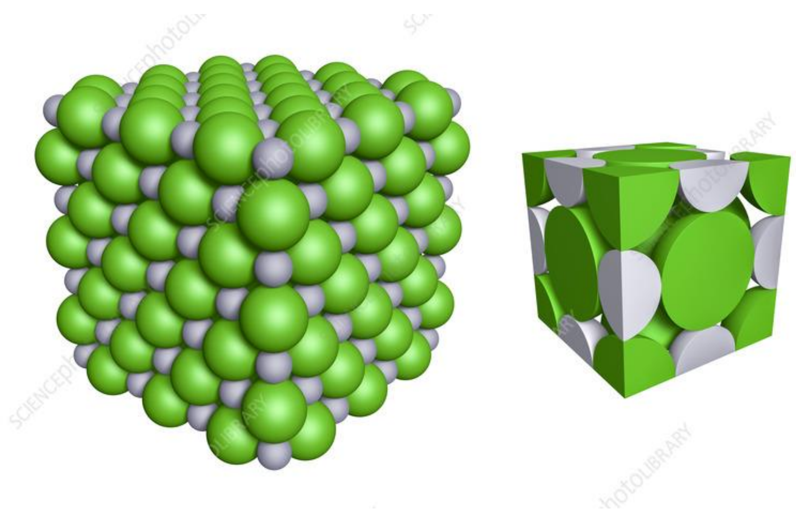


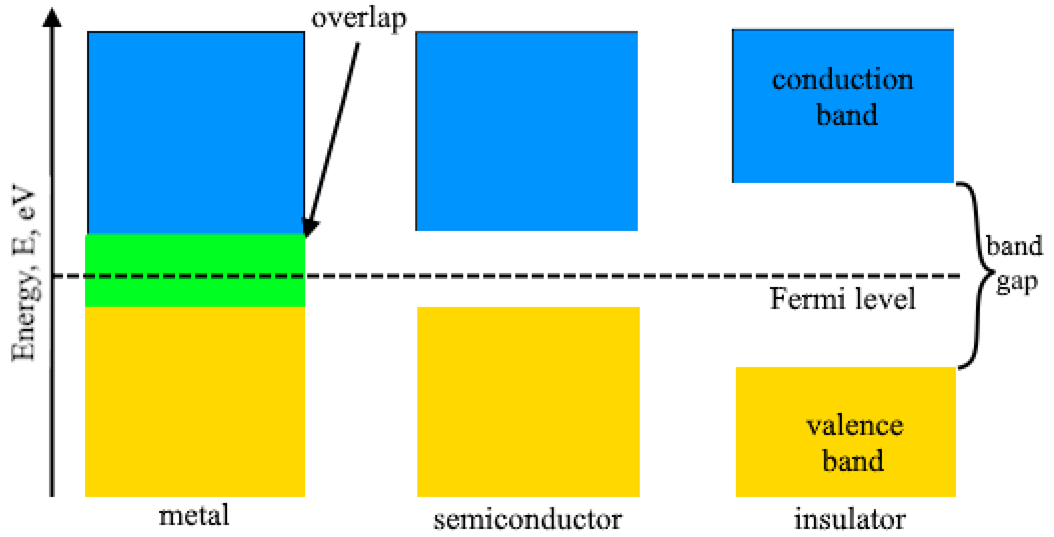
A schematic diagram of the Ge NP solar cell.



III. Peculiarities of the structure and properties of semiconductor nanomaterials

Solid materials

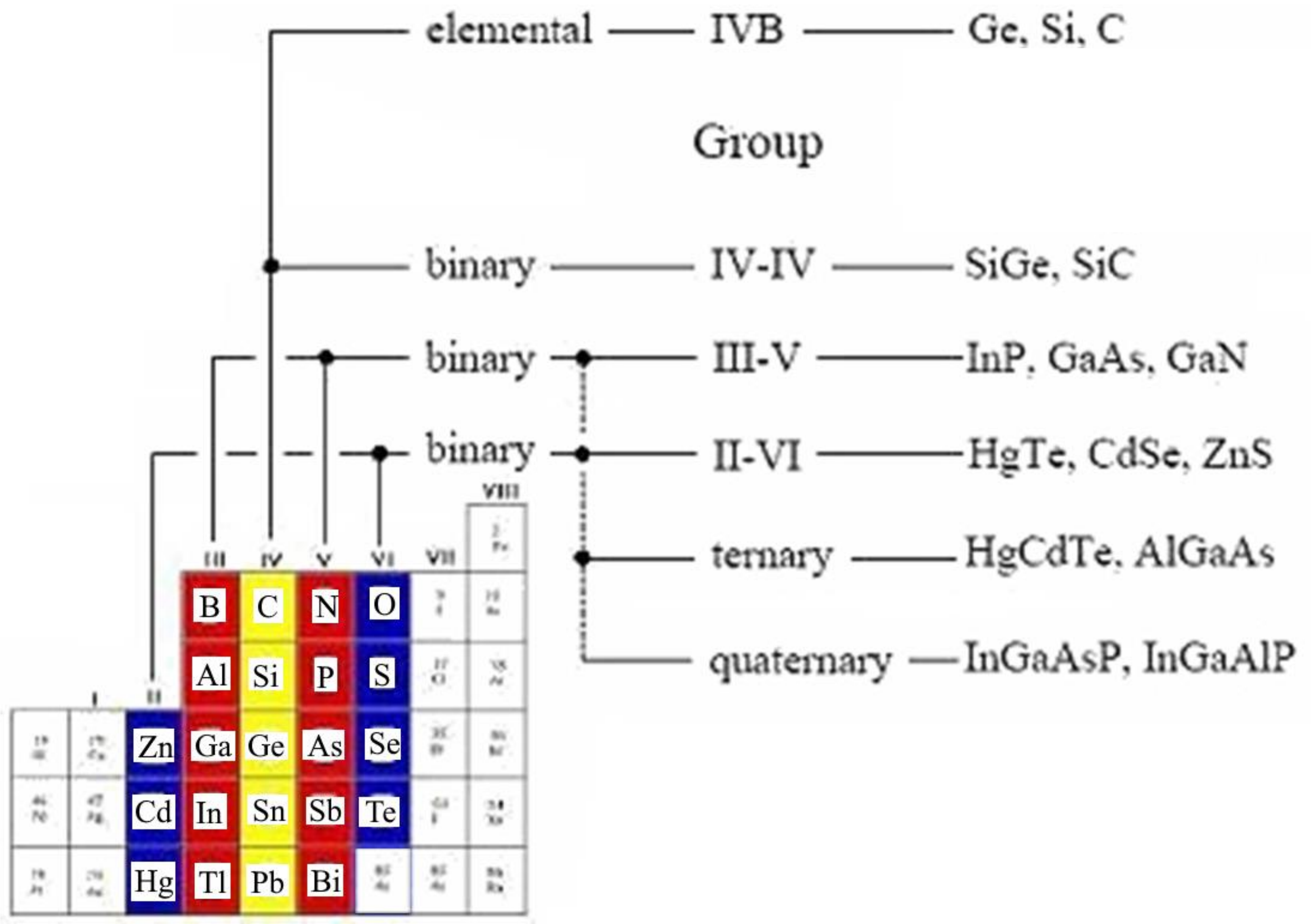




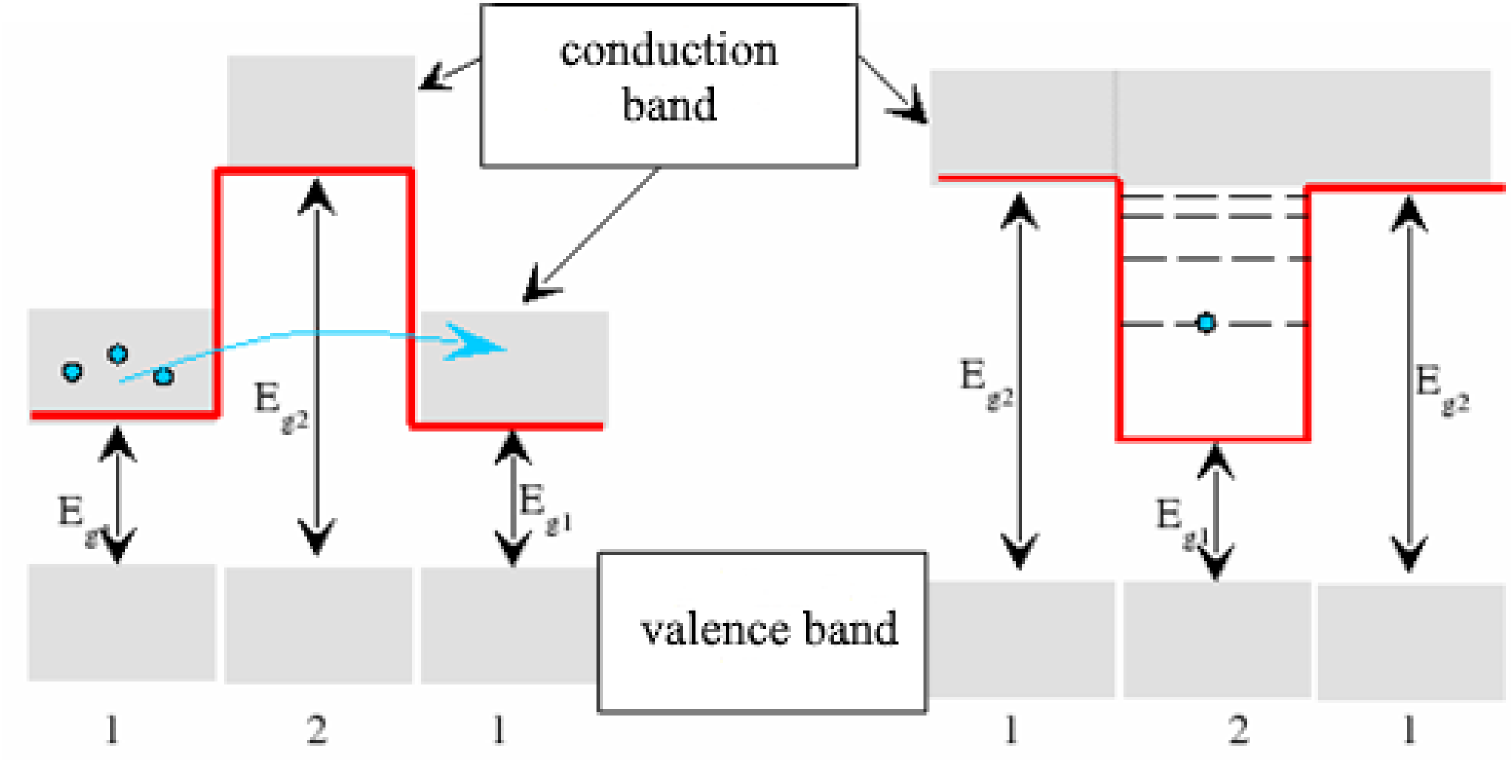
A diagram showing the valence and conduction bands of insulators, metals, and semiconductors. The Fermi level is the name given to the highest energy occupied electron orbital at absolute zero.

Kumar, D. S., Kumar, B. J., & Mahesh, H. M. (2018). Quantum nanostructures (QDs): an overview. *Synthesis of inorganic nanomaterials*, 59-88.

Semiconductor materials



Multilayer solar cells' band structure



(a) (b)

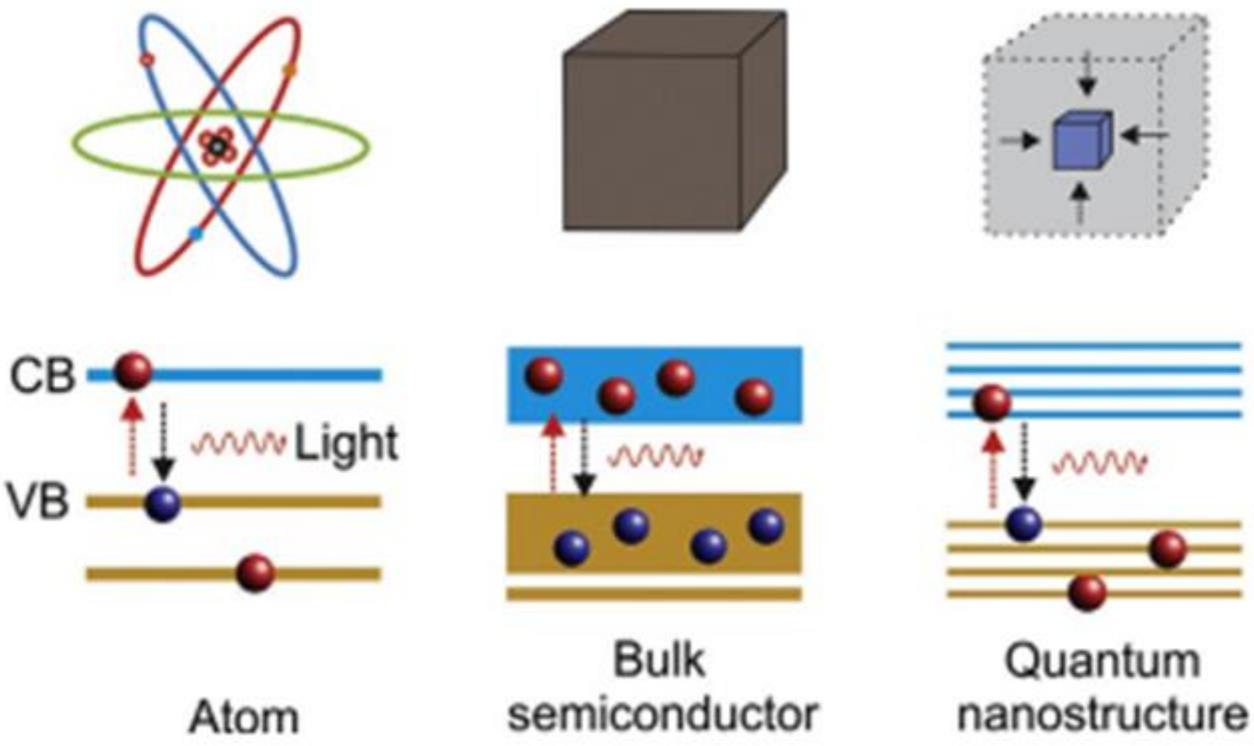
Formation of quantum barrier (a) and quantum well (b).

The allowed energy levels in the quantum well:

$$E = \frac{mv^2}{2} = \frac{p^2}{2m} = \frac{h^2}{2m\lambda^2} = \frac{h^2}{8ml^2}n^2$$

where p is the electron momentum, m is its mass, h is Planck's constant.

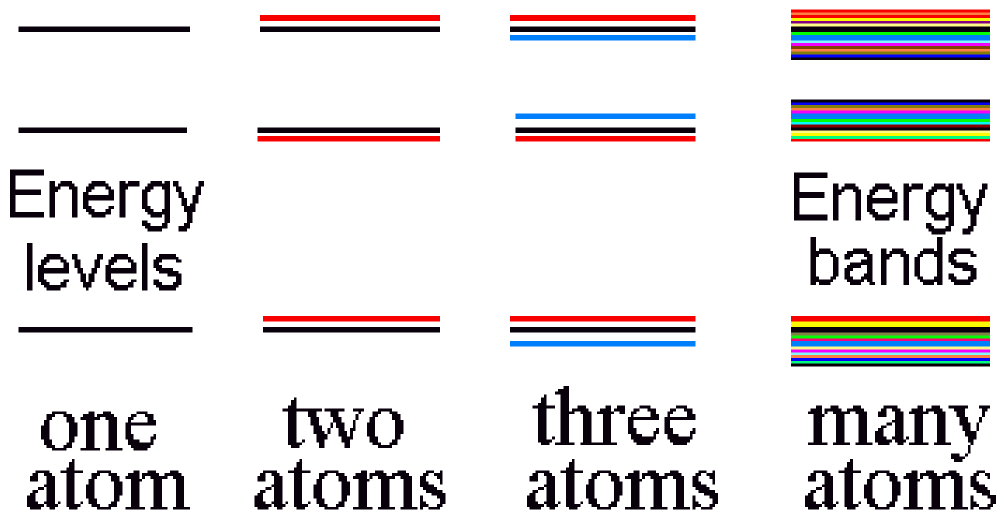
Size dependency of energy band structure

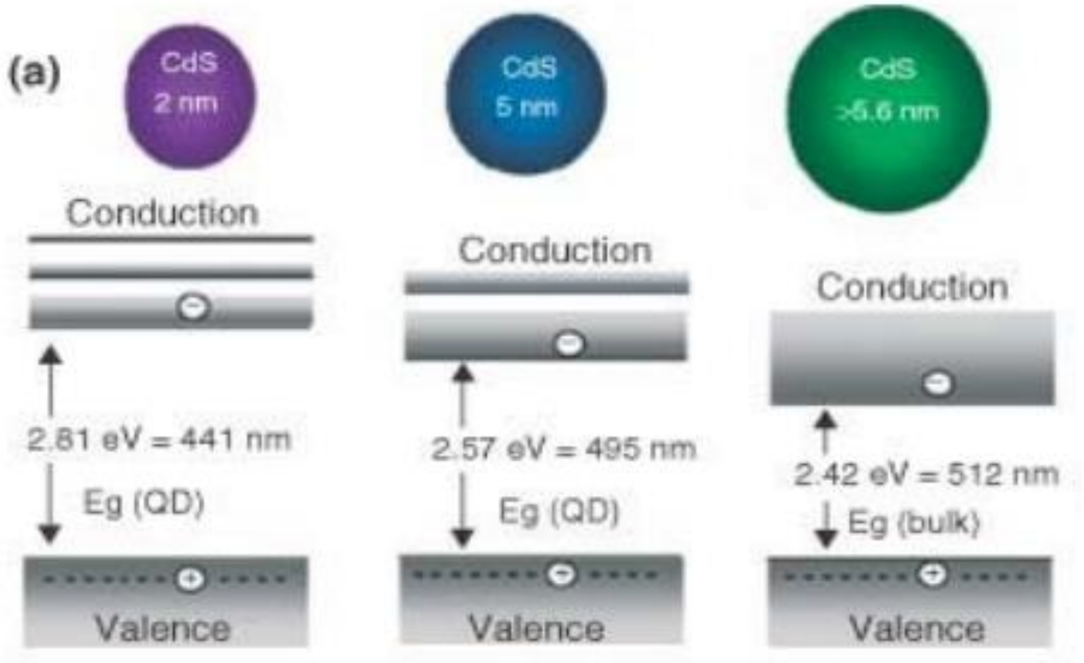


Schematic diagram of the energy band structure in atom, bulk structure and nanomaterial

Kumar, D. S., Kumar, B. J., & Mahesh, H. M. (2018). Quantum nanostructures (QDs): an overview. *Synthesis of inorganic nanomaterials*, 59-88.

Size dependency of energy band structure

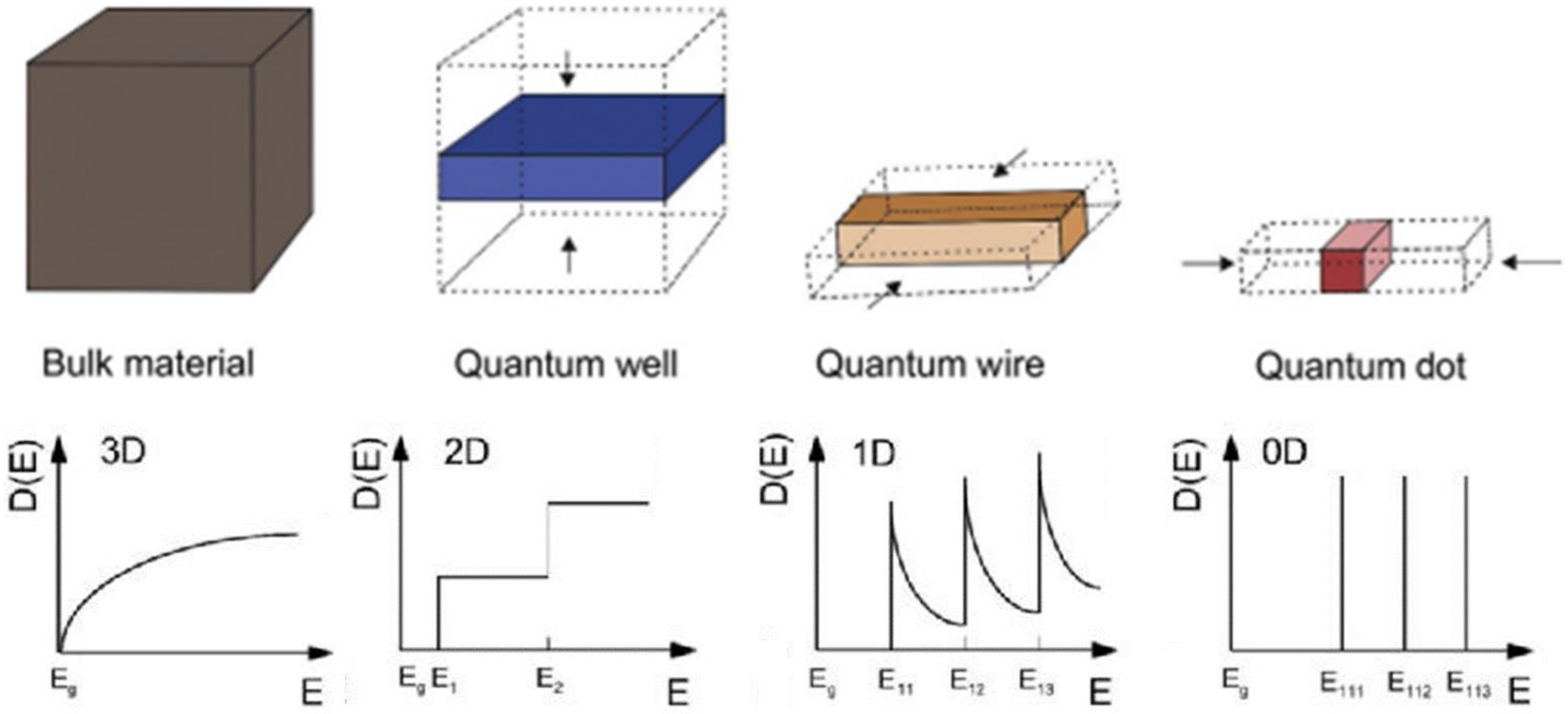




Size-dependent band gap from atom to QDs (quantum confinement model)

[https://www.physics.udel.edu/~watson/scen103/98w/clas0121c.html]
[https://www.frontiersin.org/articles/10.3389/fphy.2021.612070/full]

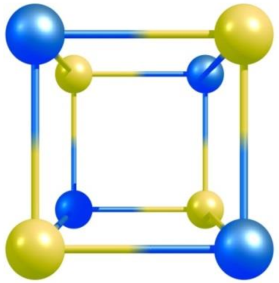
Size dependency of energy band structure

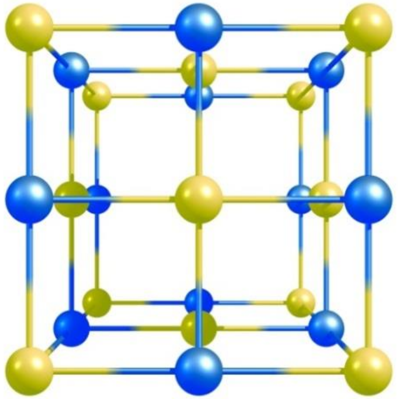


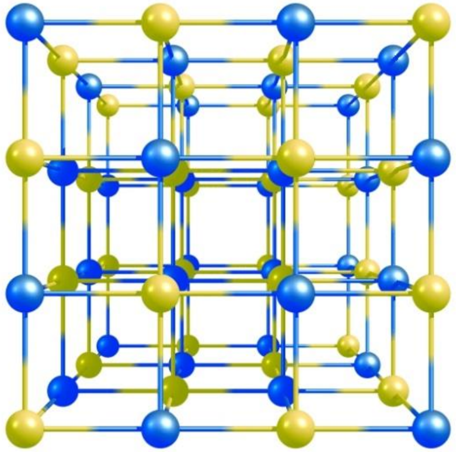
Schematic diagram for bulk material and quantum nanostructures: quantum well, quantum wire, quantum dot.

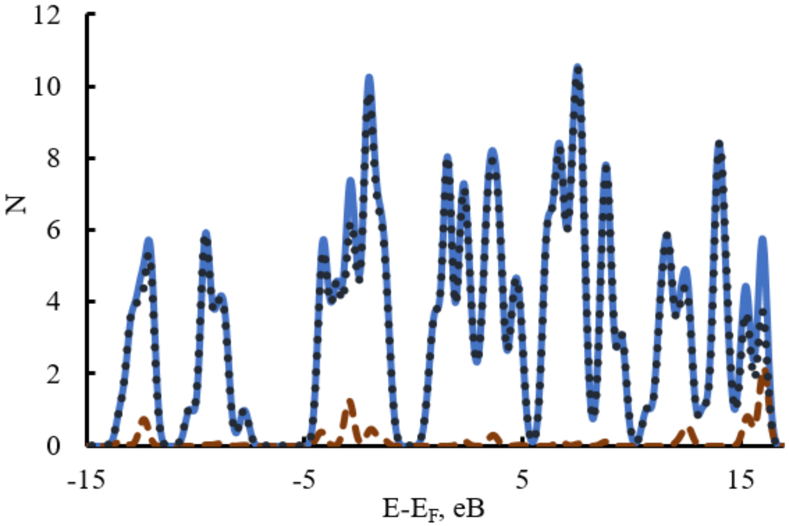
[Kumar, D. S., Kumar, B. J., & Mahesh, H. M. (2018). Quantum nanostructures (QDs): an overview. *Synthesis of inorganic nanomaterials*, 59-88];
[http://org.ntnu.no/solarcells/pages/pn-junction.php]

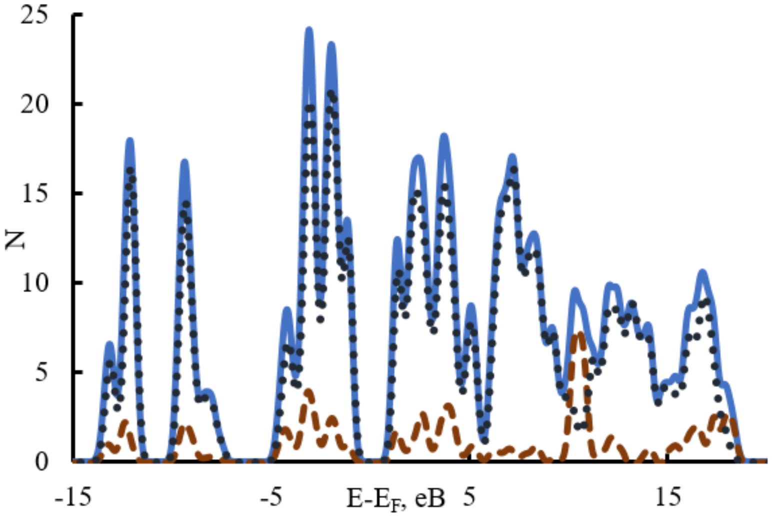
Band structure of PbTe





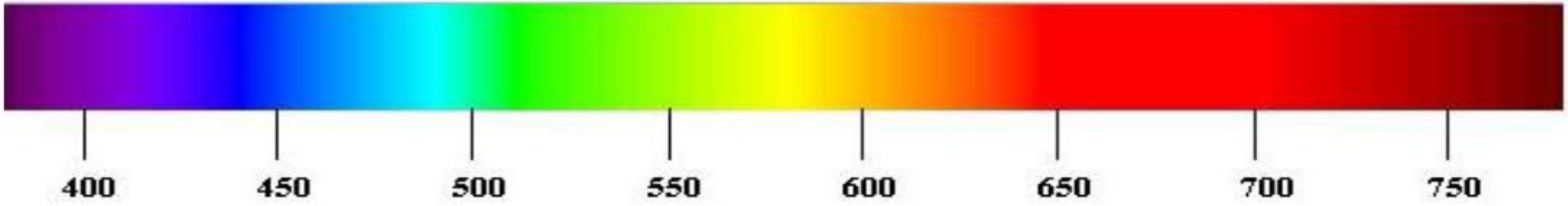




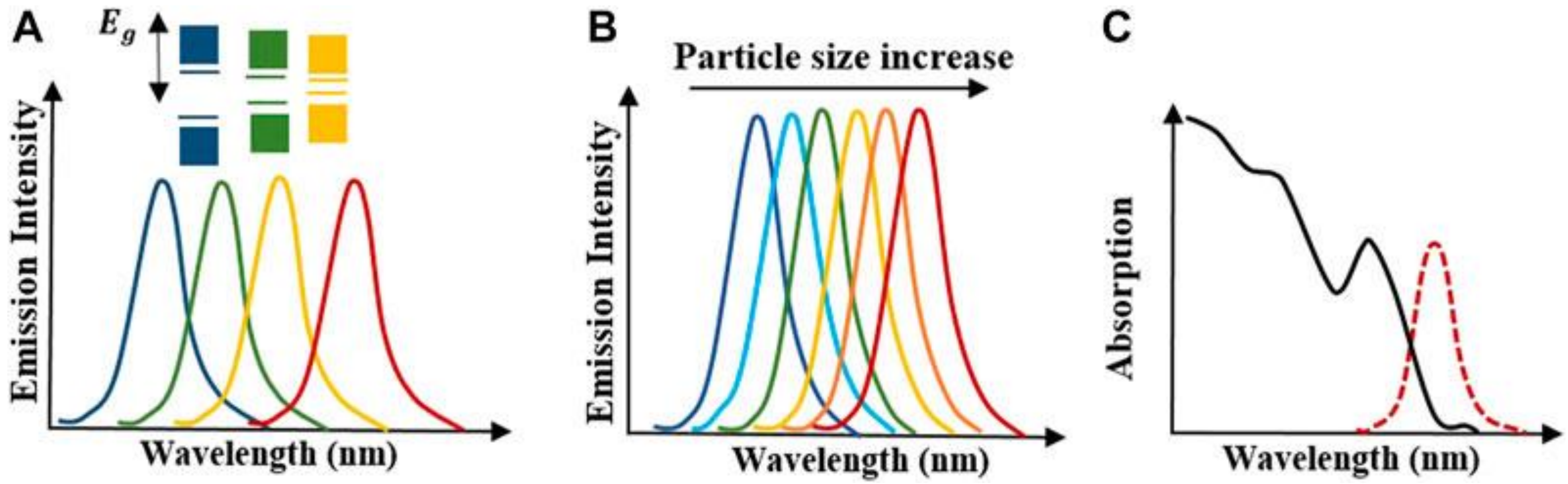


Density of electronic states of clusters: a) $Pb_{14}Te_{13}$, b) $Pb_{32}Te_{32}$ Solid line - total values, dots - contribution of surface atoms, dashed line - contribution of internal atoms in DOS.

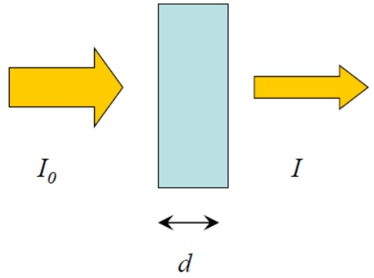
Absorption of light



Wavelength, nm



Bouguer-Lambert law :



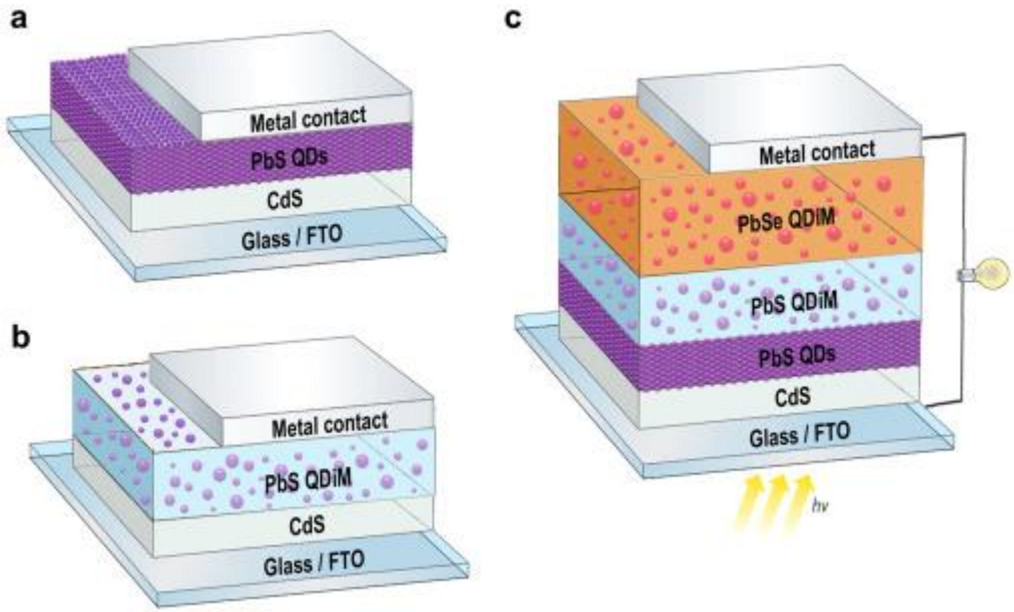
$$d \to 0; I \to I_0$$

$$I = I_0 e^{-kd}$$

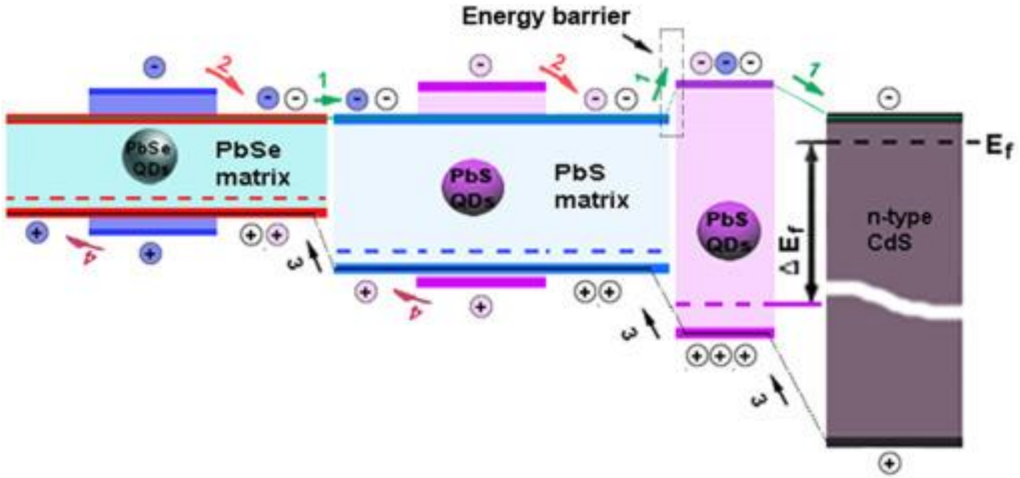
[Kalsoom UE, et. al. (2021). Nonlinear optical properties of CdSe and CdTe core-shell quantum dots and their applications. *Frontiers in Physics*, *9*, 612070.]

REGINNA 4.0

3rd generation: tandem solar cells



Schematic illustration of CBD-PbS/CdS solar cells with different assembled structures. (a) Traditional PbS-QDs/CdS solar cell, (b) PbS-QDiM/QDs/CdS stacked tandem two-layer solar cell and (c) PbSe-QDiM /PbS-QDiM/QDs/CdS stacked tandem triple-layer solar cell.



[https://doi.org/10.1002/wnan.78]

Techniques for nano-size materials investigation

Transmission electron microcopy

Energy dispersive X-ray Spectroscopy (TEM)

Scanning electron microcopy

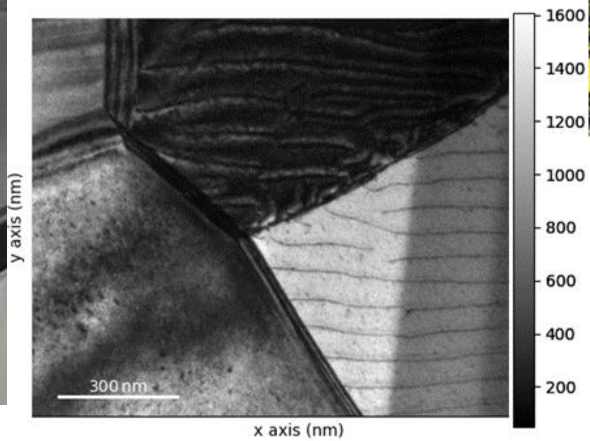
X-ray Diffraction

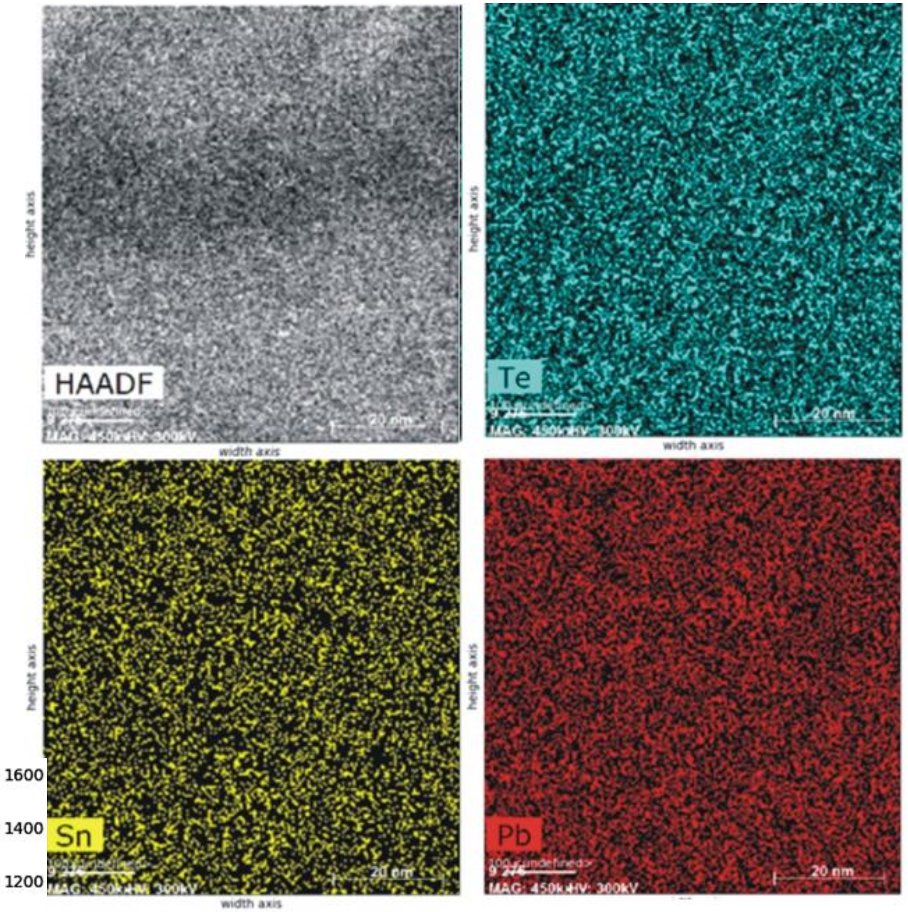
Atomic Force Microscopy (AFM)

Thermoelectric properties investigation

Photovoltaic measurements

SEM application for surface structure analysis

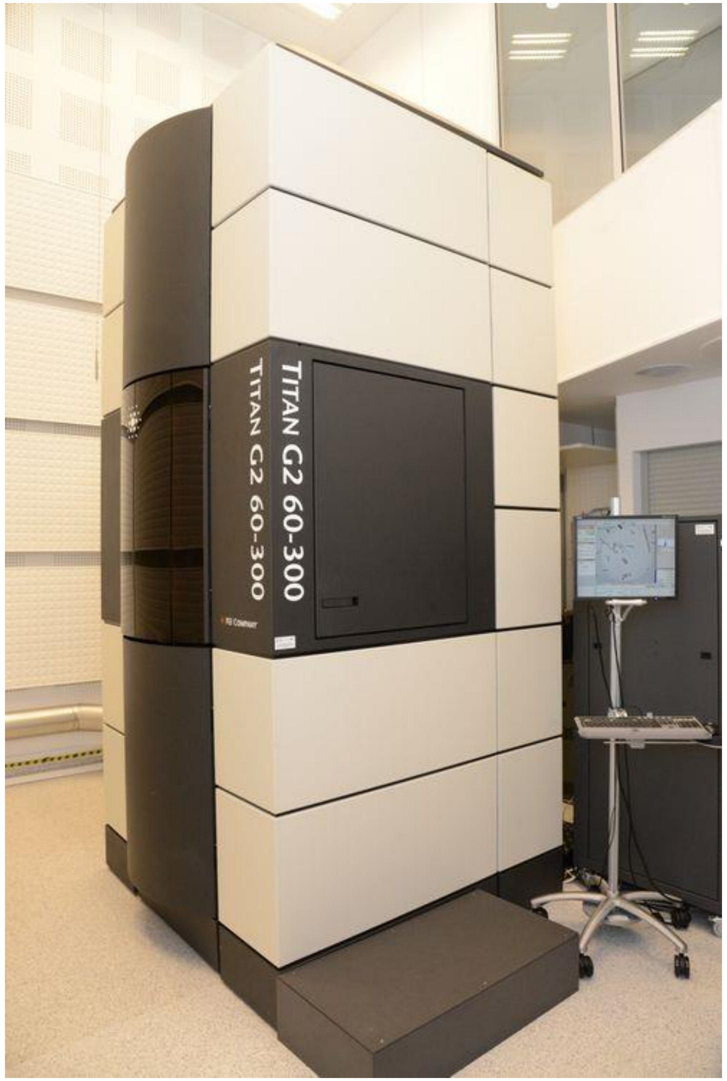


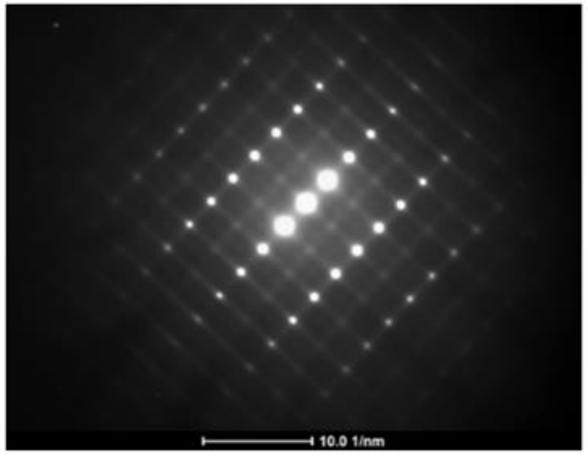


EDX maps of elemental distribution.
Scale: 20 nm.

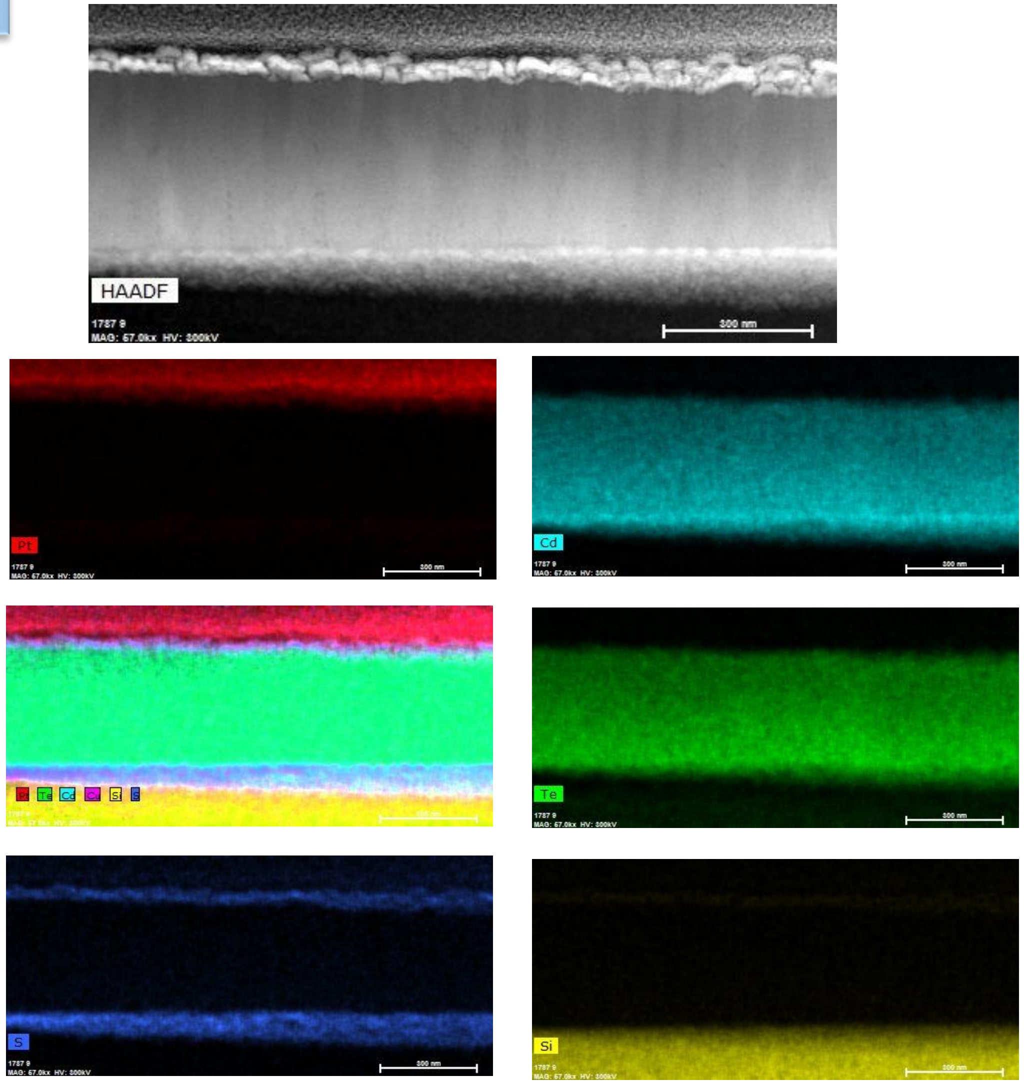
[Saliy Y. et al. (2023). *Physics and Chemistry of Solid State*, *24*(1), 70-76.]

Transmission Electron Microscope



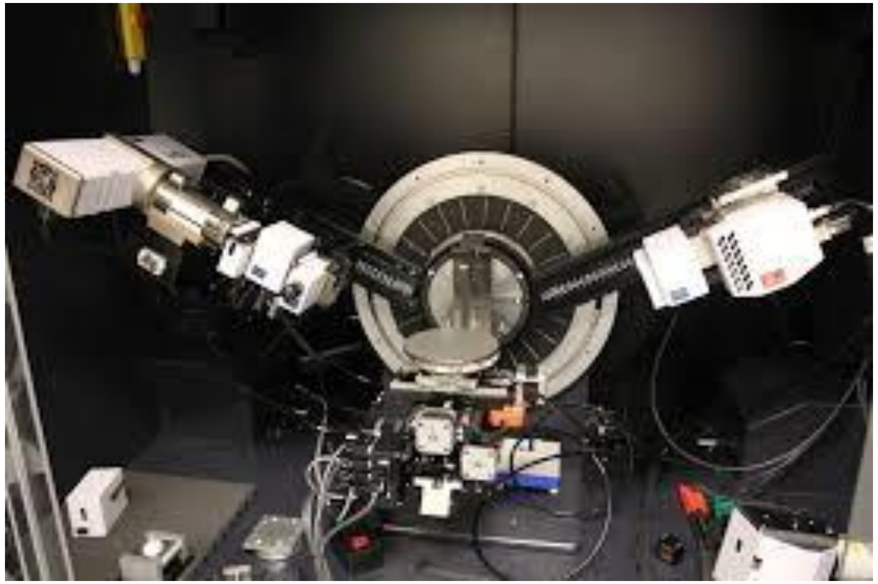


Transmission electron microscopy image of diffraction of crystalline material.



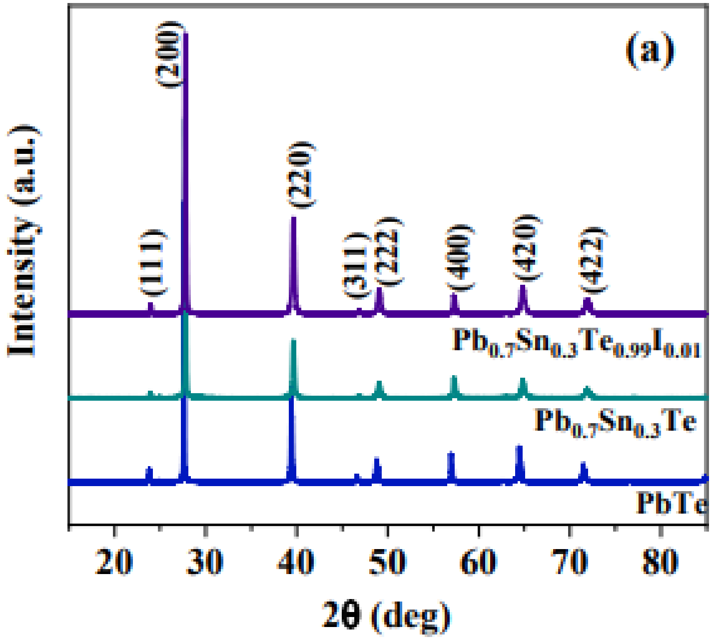
EDX distribution map for the multilayer Si/Cu/CdS/CdTe specimen.

X-ray Diffraction Analysis



Apparatus	Bruker Discover D8
Function	Structure characterization
Main Purpose	X-Ray Diffraction analysis of thin films
Main Characteristics	High resolution XRD

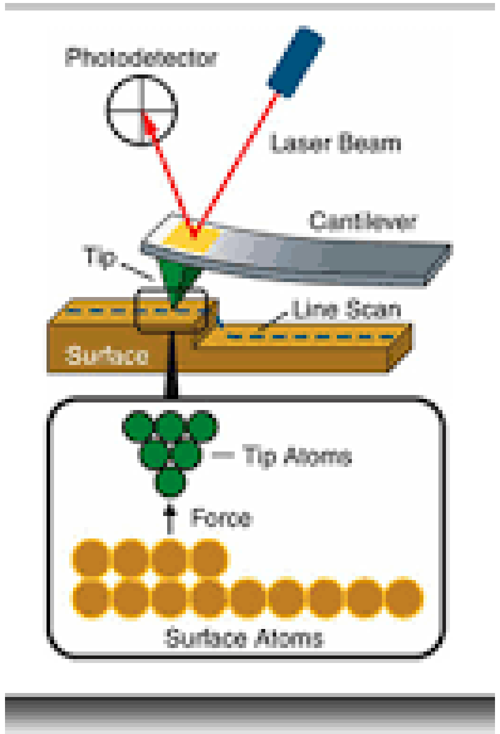
Facilities	X-ray reflectometry, grazing angle diffraction, stress analysis, texture analysis, x-y mapping, reciprocal space mapping
Specimen	Flexible, max 80 x 50 x 20 mm



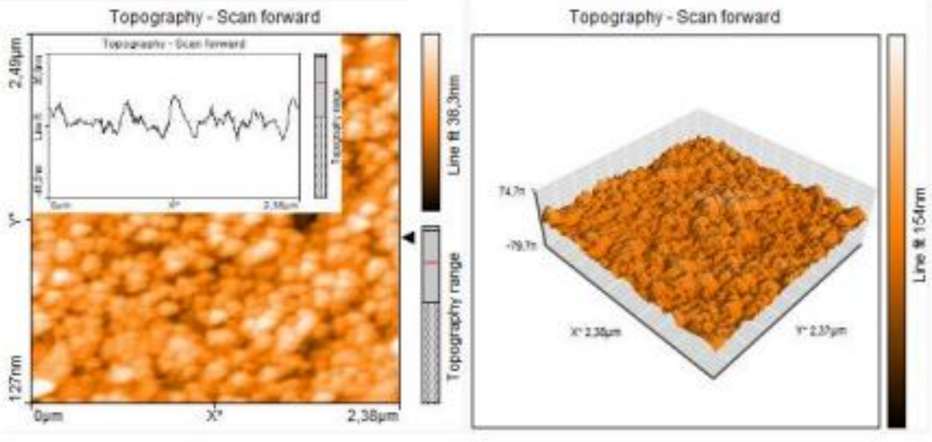
The powder X-ray diffraction patterns for PbTe, $Pb_{0.7}Sn_{0.3}Te$, and $Pb_{0.7}Sn_{0.3}Te_{0.99}I_{0.01}$ specimens.

[Saliy Y. et al. (2023). *Physics and Chemistry of Solid State*, *24*(1), 70.]
[https://www.tudelft.nl/en/faculty-of-applied-sciences/about-faculty/departments/quantum-nanoscience/kavli-nanolab-delft/equipment/inspection/bruker-xrd]

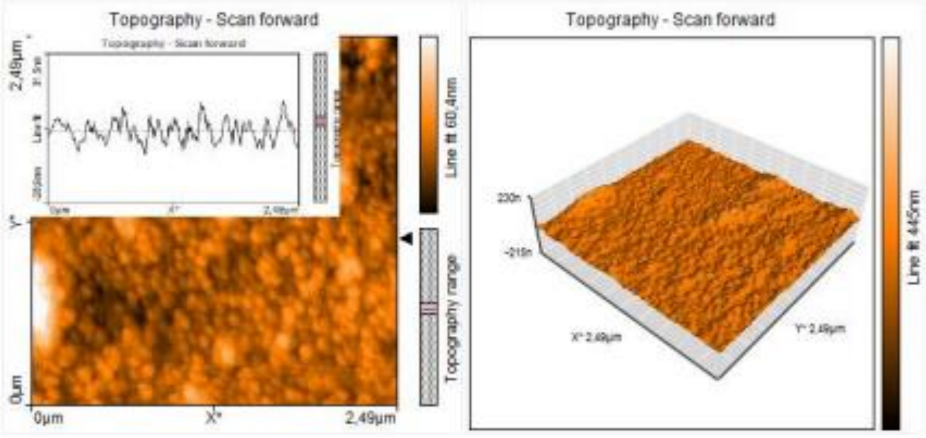
Atomic Force Microscopy (AFM) analysis



[Saliy YP, et.al. (2017) Journal of Nano and Electronic Physics.9(5). p. 05016.]
[Agarwal DH, et. al. (2012, June). Development of portable experimental set-up for AFM to work at cryogenic temperature. In AIP Conference Proceedings (Vol. 1447, No. 1, pp. 531-532).]



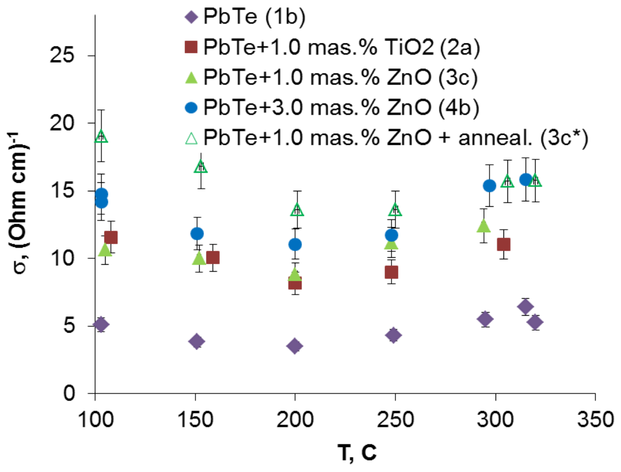
a

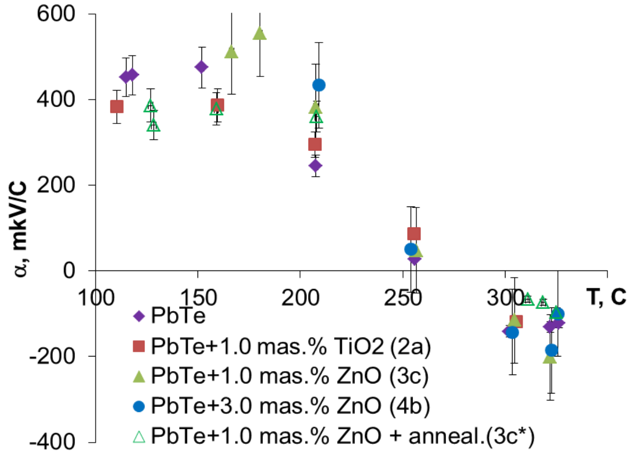


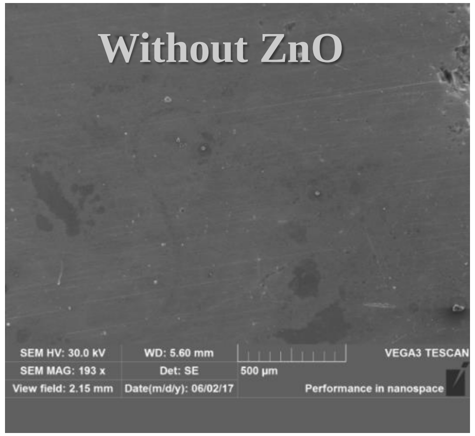
b

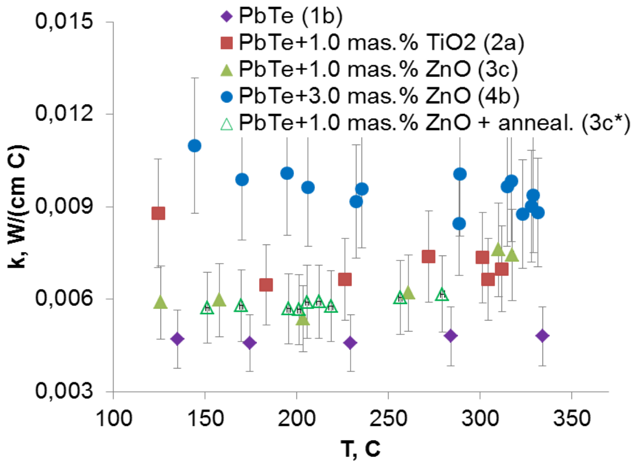
AFM images of the CdTe films, deposited on glass with thick (a) and thin (b) thickness.
The size of the observed surface is 2.5 x 2.5 micron^2.

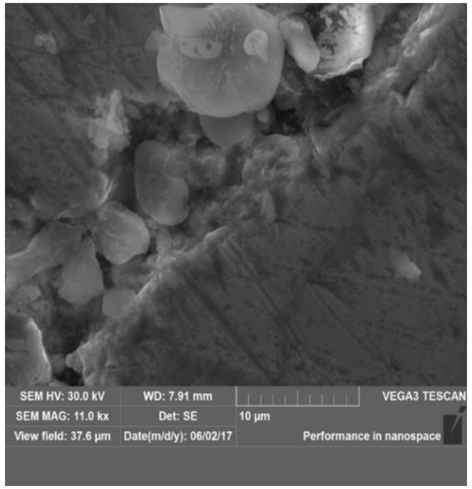
Thermoelectric parameters (PbTe: ZnO)

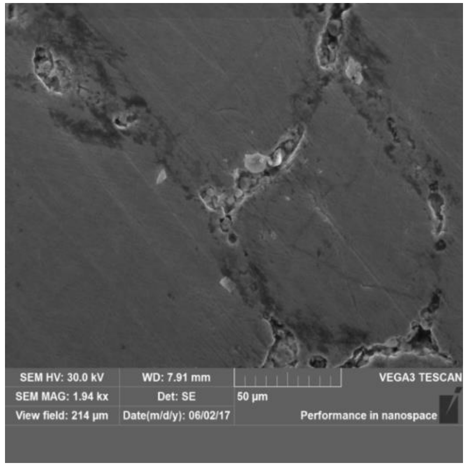


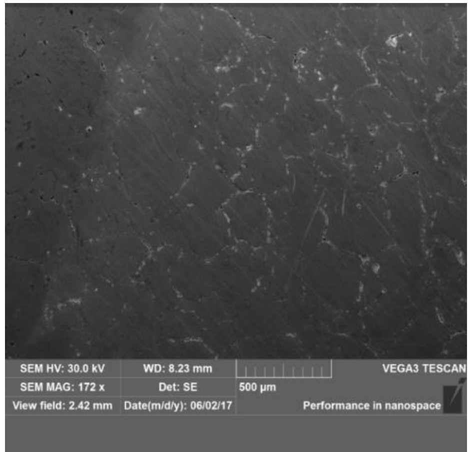






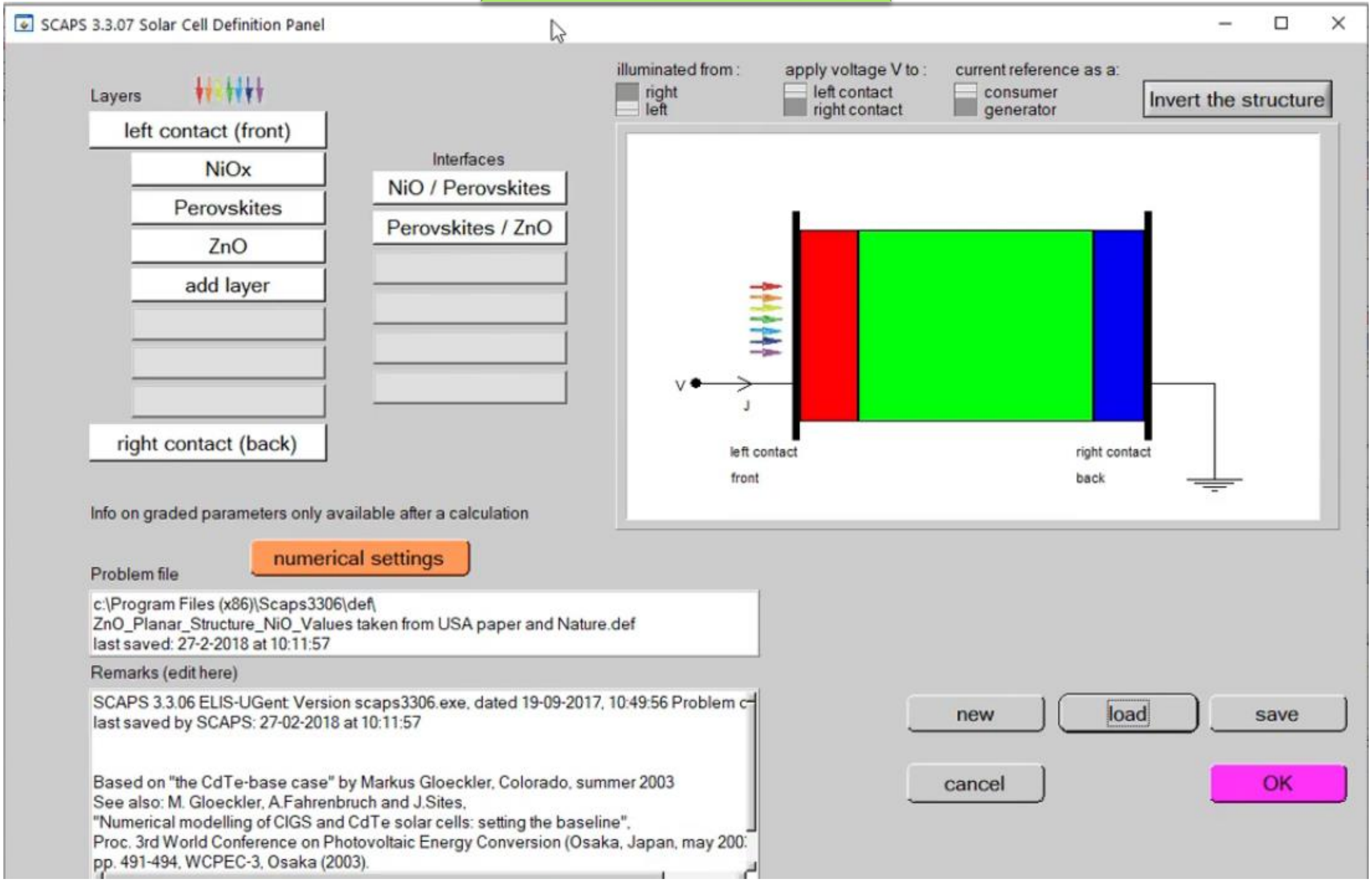


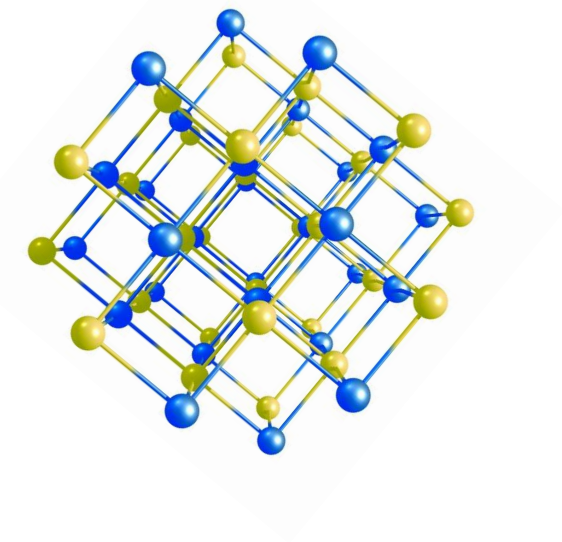




Temperature dependence of specific conductivity σ (a), thermoelectric coefficient α (b) and thermal conductivity *k* (c) of PbTe samples with the ZnO impurities (nanodispersed powders). For all samples: PbTe fractions of (0.05-0.5) mm, pressing pressure of 1.5 GPa. The sample 3c* was additionally annealed for 15 minutes at 500 °C.

Theoretical modelling





IV. Practical application of nanomaterials

Photovoltaic power station

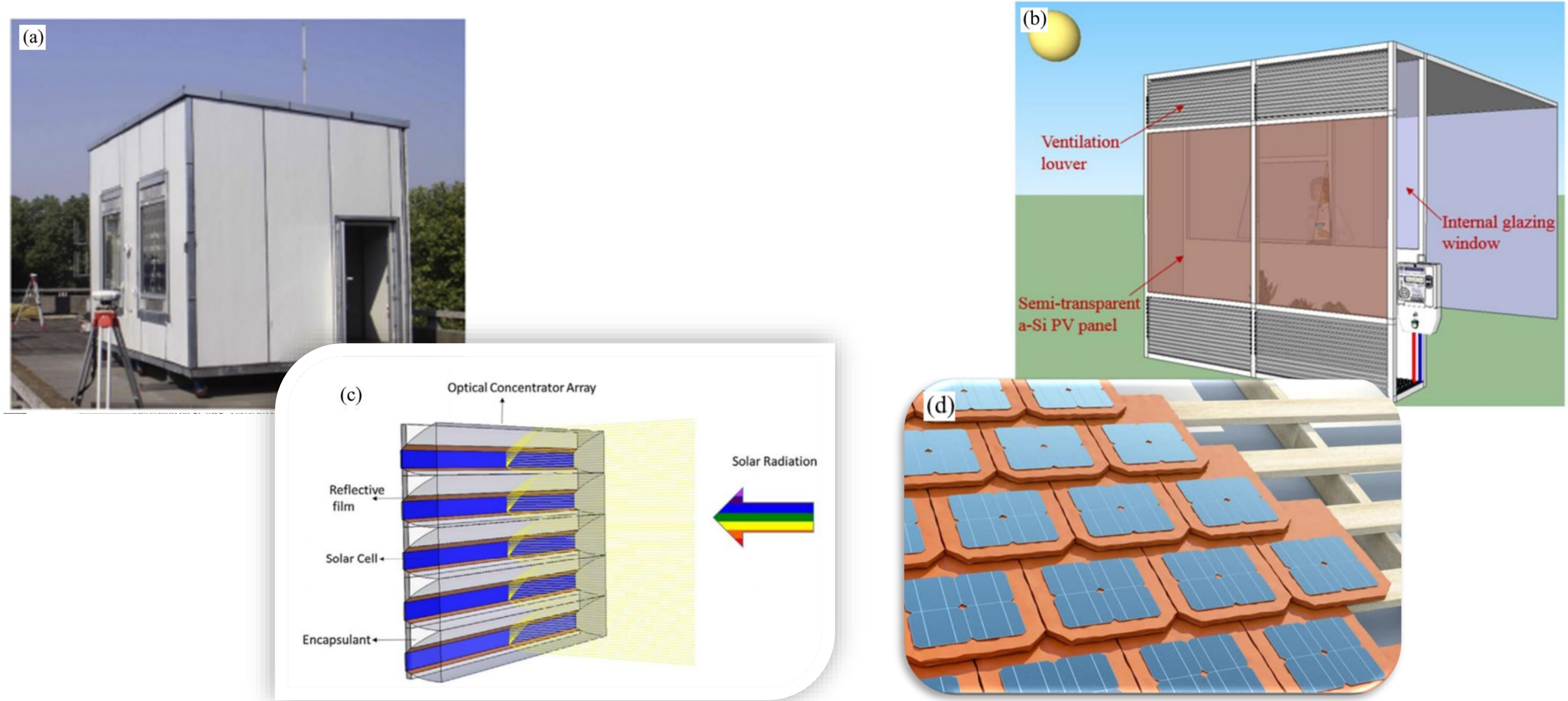
Solar power satellites

[https://www.shutterstock.com/search/solar-power-satellite]

Photovoltaic cover

[Li X., et al. (2021). Review and perspective of materials for flexible solar cells. Materials Reports: Energy, 1(1), 100001.]

Photovoltaic surfaces for buildings

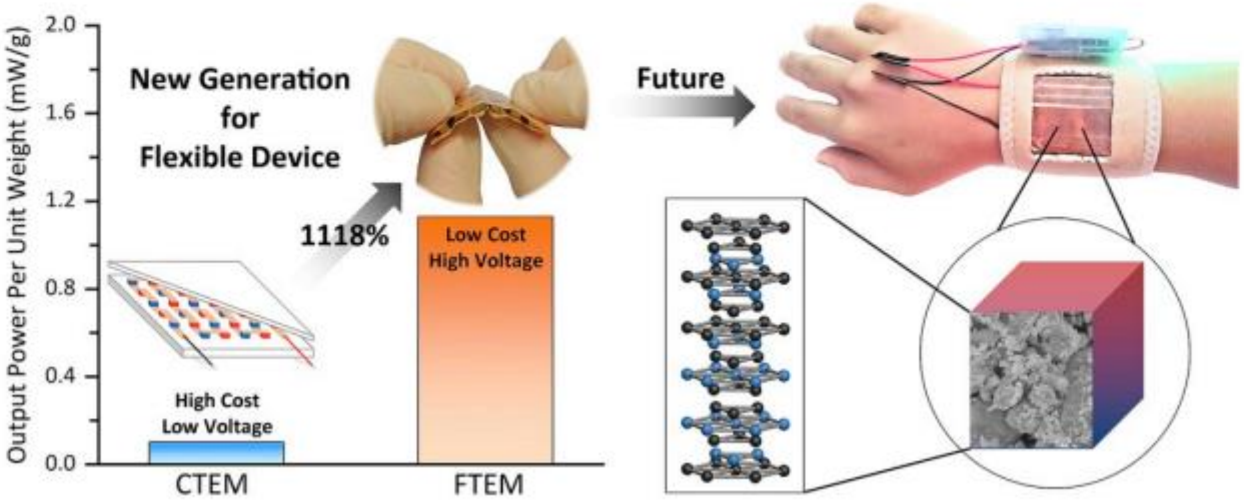


A ventilated semi-transparent photovoltaic (PV) façade (a) and a photovoltaic double-skin façade (b), a building-integrated concentrating photovoltaic (c), roof panels (d).

[Zhang T. et.al. Energies 2018, 11, 3157]; [https://solarmagazine.com/solar-panels/]

Thermoelectric devices for everyday use

Matrix Power Watch (Boukai, 2017)



Conventional thermoelectric modules (CTEMs),
Flexible thermoelectric modules (FTEMs)

[http://www.sel.eesc.usp.br/jcarmo/pdfs/PUBLICACOES/CAPITULOS/CAP07.pdf]
[You HJ, et. al. (2019). Influence of different substrate materials on thermoelectric module with bulk legs. Journal of Power Sources, 438, 227055.]

Thermoelectric devices in health care devices

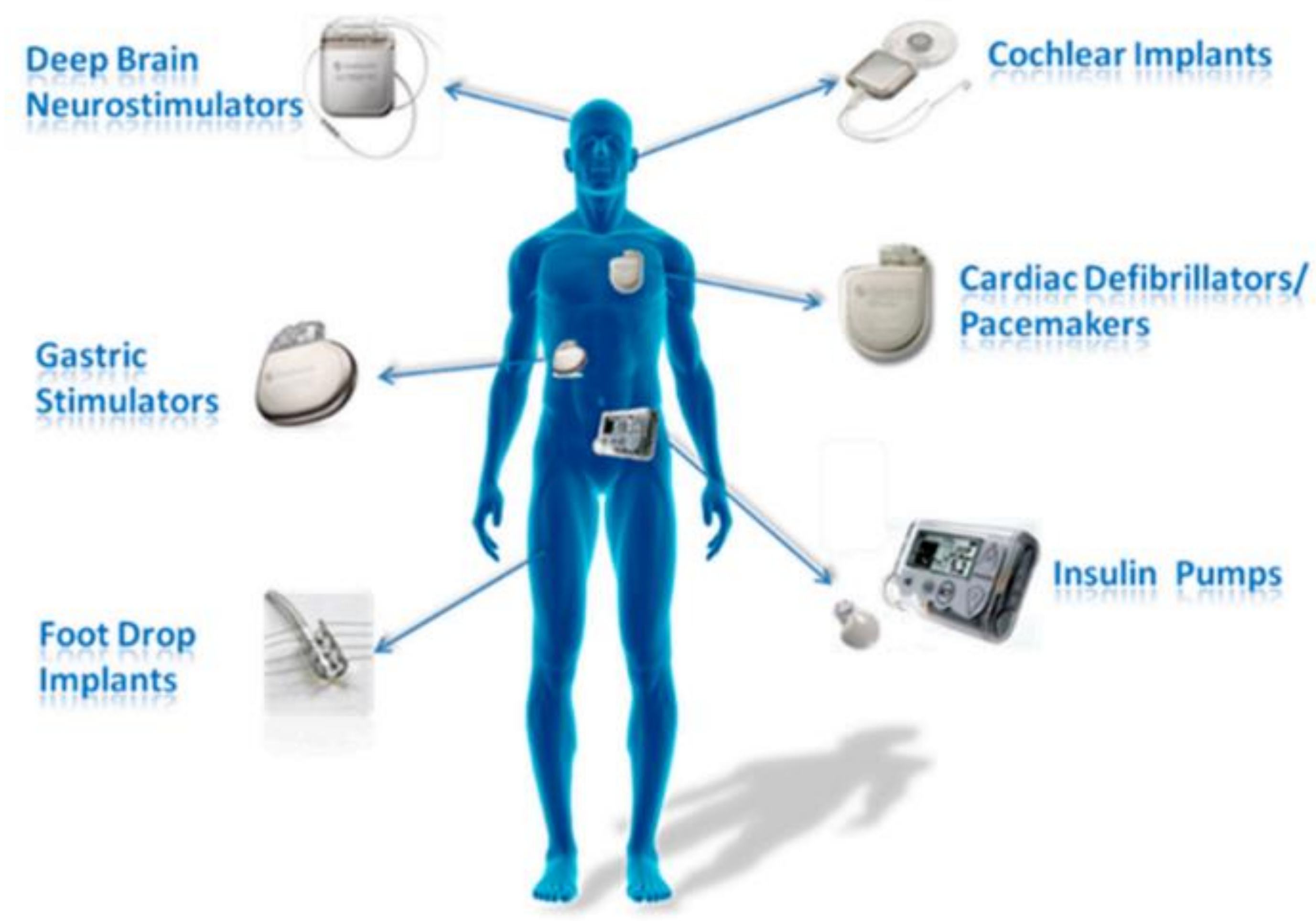


Figure 13. Common implantable devices.

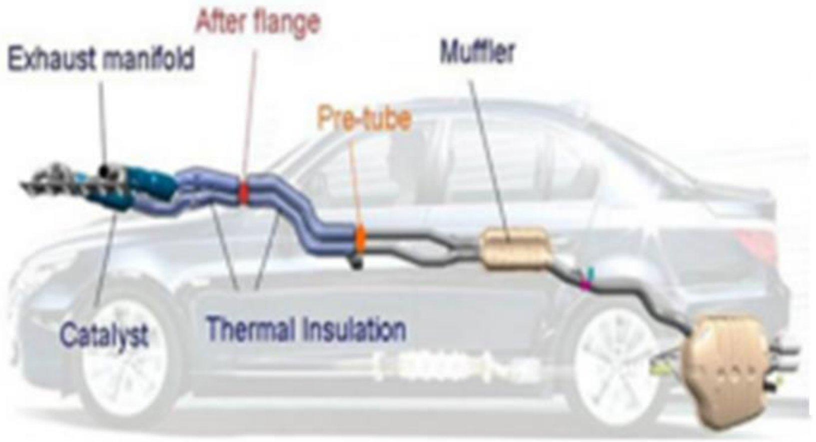
[Kumar et al. (2019). The design of a thermoelectric generator and its medical applications. *Designs*, *3*(2), 22.]

Thermoelectric devices in medicine

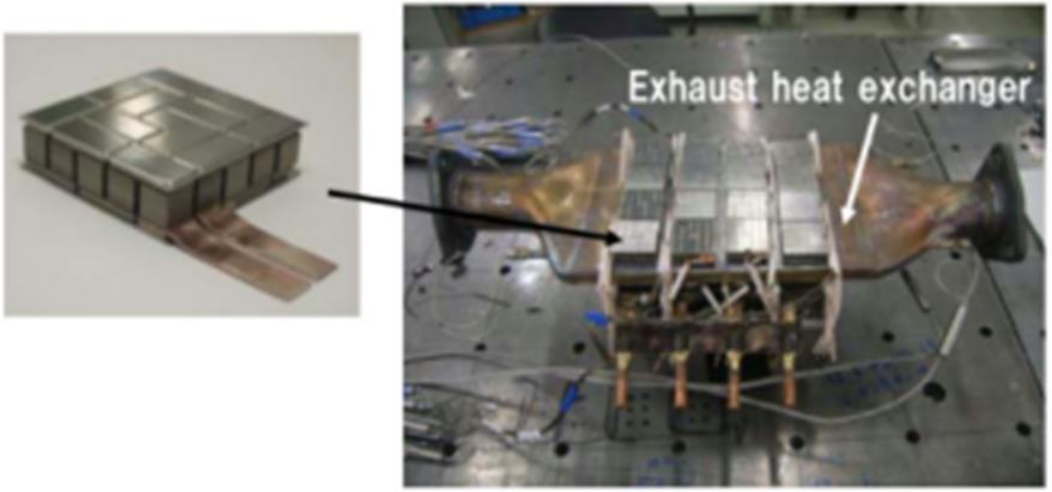
Thermoelectric projects form do IMEC; (a) Pulse oximeter powered by a TEG with power consumption of 62 µW at 22ºC; (b) Body-powered ECG headband and (c)) electrocardiography (ECG) shirt

[http://www.sel.eesc.usp.br/jcarmo/pdfs/PUBLICACOES/CAPITULOS/CAP07.pdf],
[Leonov, V. (2013). Thermoelectric energy harvesting of human body heat for wearable sensors. *IEEE Sensors Journal*, *13*(6), 2284-2291.]

Thermoelectric devices in car mechanisms

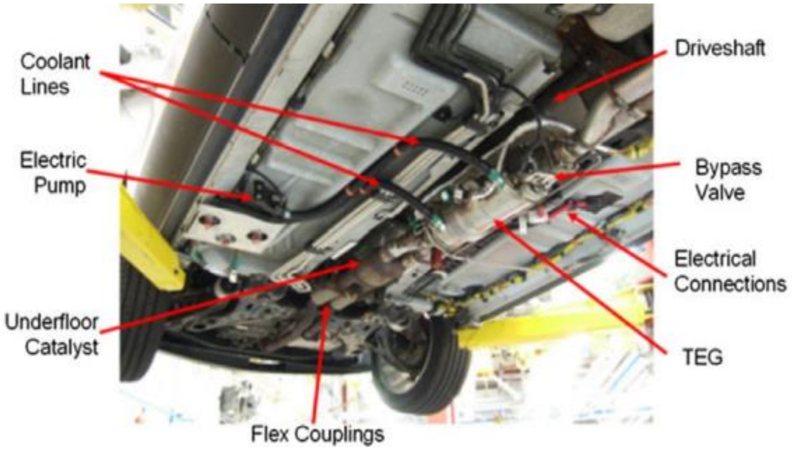


(a)



(b)

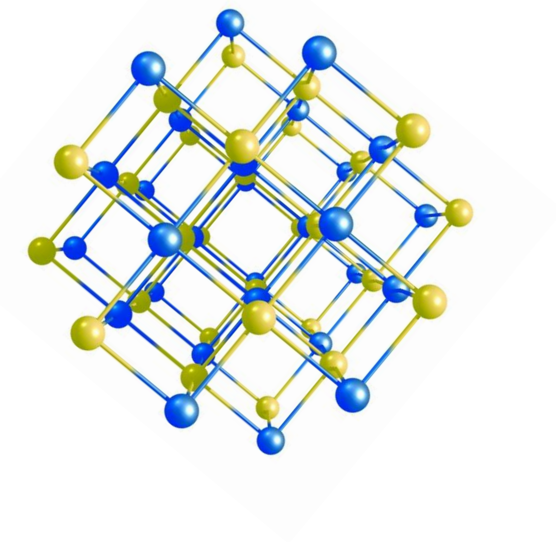
Thermoelectric generator’s positions: (a) Exhaust system inside a passenger vehicle (Crane and LaGrandeur, 2010). (b) TEG’s assembly on a flat heat exchanger (Mori et al., 2011)



Integration of the TEG into the underfloor of the Ford Lincoln MKT vehicle

[Crane D., et al. TEG On-Vehicle Performance and Model Validation and What It Means for Further TEG Development. *J. Electron. Mater.* **42**, 1582–1591 (2013).]

REGINNA 4.0



V. Exercises: Characterization of nanomaterials

1) Select a scenario of interest for you:

electronic devices of a small airplane

kitchen equipment

touristic camping

doctors’ tablet or laptop

sports equipment

the “most popular” device

2) Where could an additional power source be useful in your chosen scenario?

3) For your report, lookout for answers to:

- Prerequisites: Description of needed materials (e.g., chemical formula, space dimensions)

- Production: What equipment do you need to obtain the sample/material needed in the device?

- Measurement and Modeling: How can you check the parameters of the device?

- Details in your chosen scenario: Where should this device be placed?

Thanks for your attention!

Bohdana NAIDYCH

bohdana.naidych@pnu.edu.ua

Supported by

eit Manufacturing

Funded by the European Union

EIT HEI Initiative