Nanomaterials Spectroscopy and Imaging

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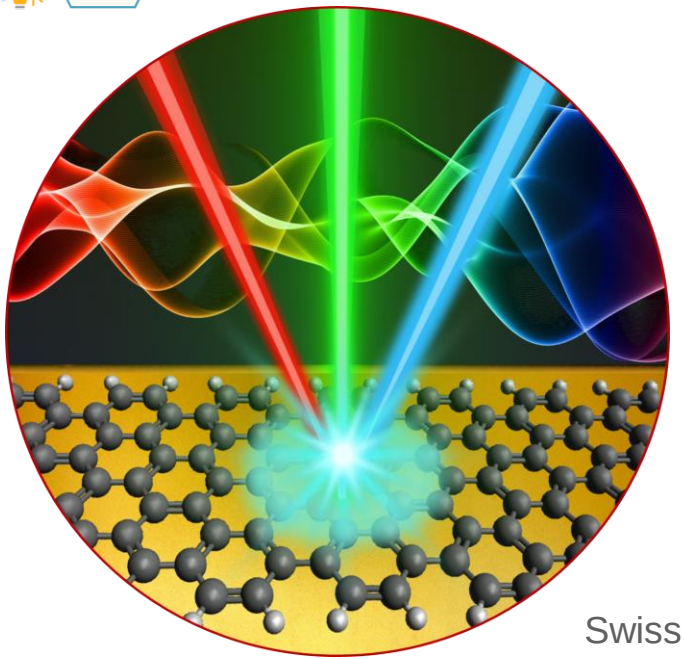

Raman spectroscopy tutorial

Mirjana Dimitrievska

Transport at Nanoscale Interfaces Laboratory

Swiss Federal Laboratories for Material Science and Technology (EMPA)

Switzerland

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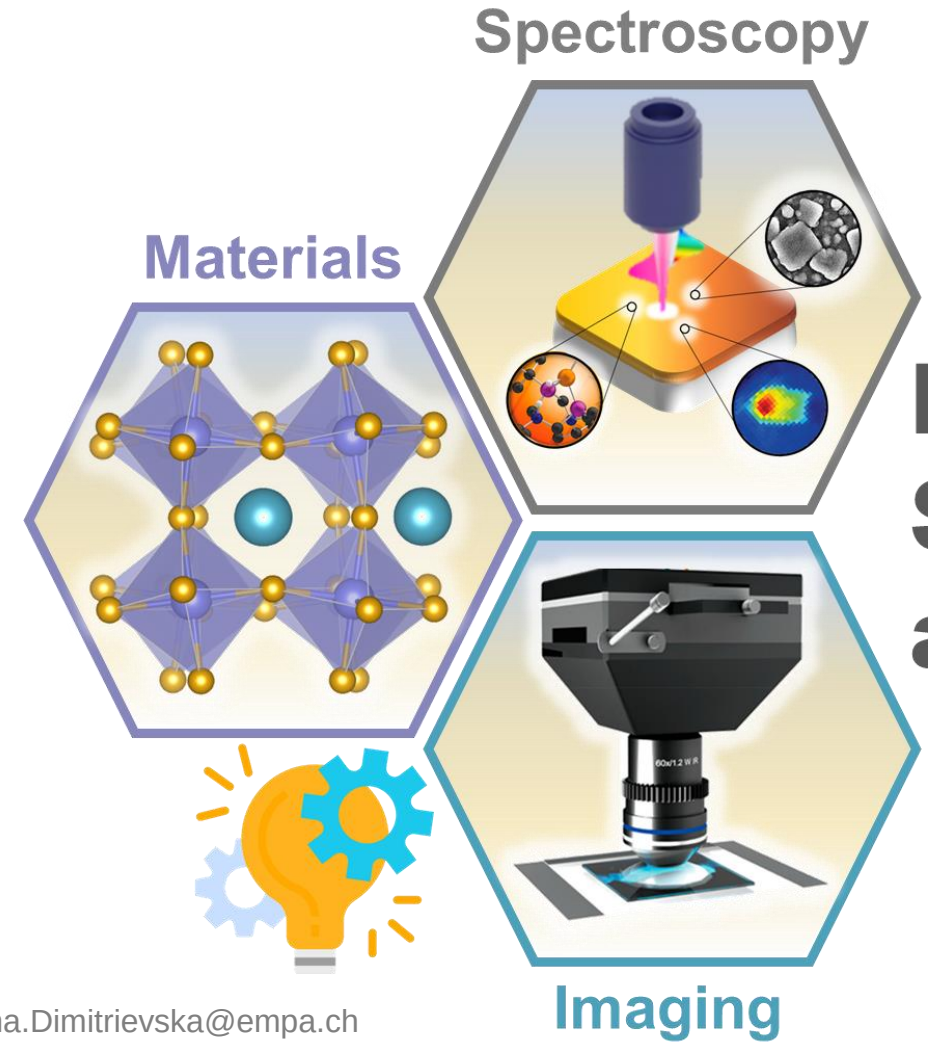

Nanomaterials Spectroscopy and Imaging

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(405) Transport at Nanoscale Interfaces

Nanomaterials Spectroscopy and Imaging Group

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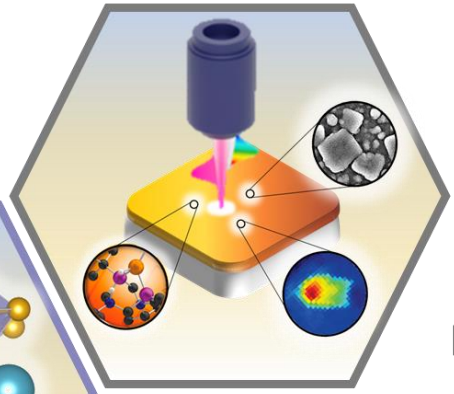
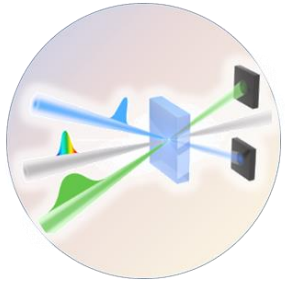
Spectroscopy

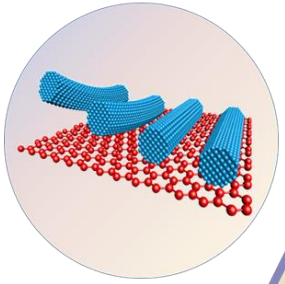


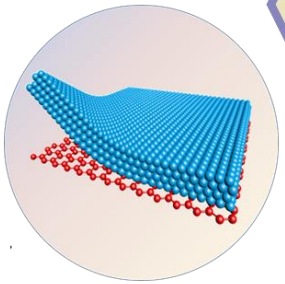
Raman, Photo-luminescence, Terahertz



Time-resolved spectroscopy, **Stimulated Raman** spectroscopy

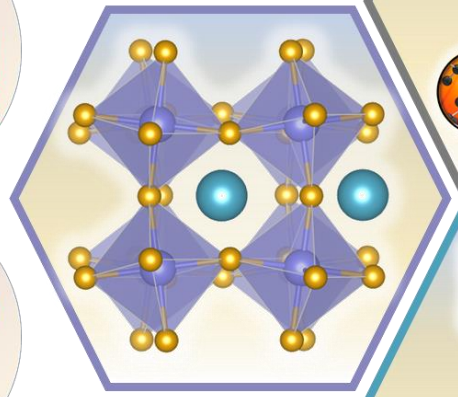
1D-2D

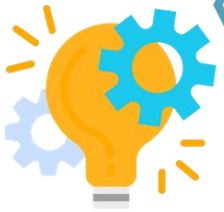




Thin films

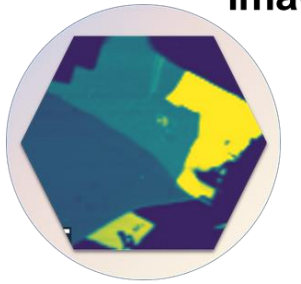
Materials

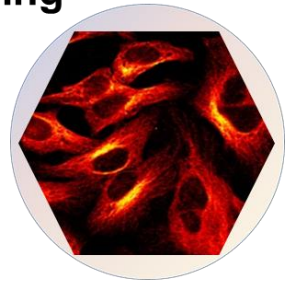




Imaging

Nanoscale label free imaging





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Let's start with atoms!

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Atoms

People

(most) Atoms like to bond!

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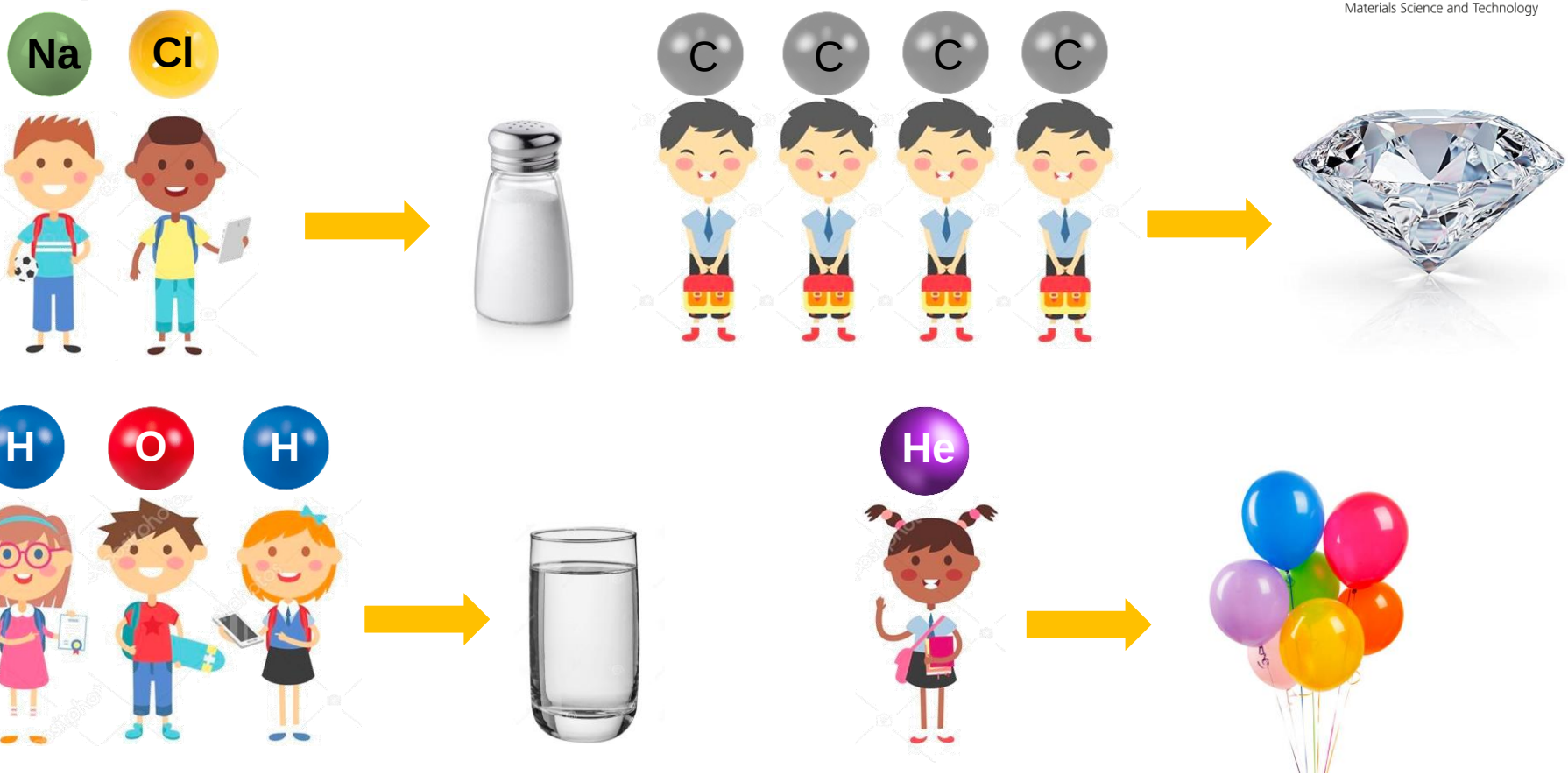

M. Dimitrievska,
Workshop “Dancing with molecules”

Atoms like to dance!

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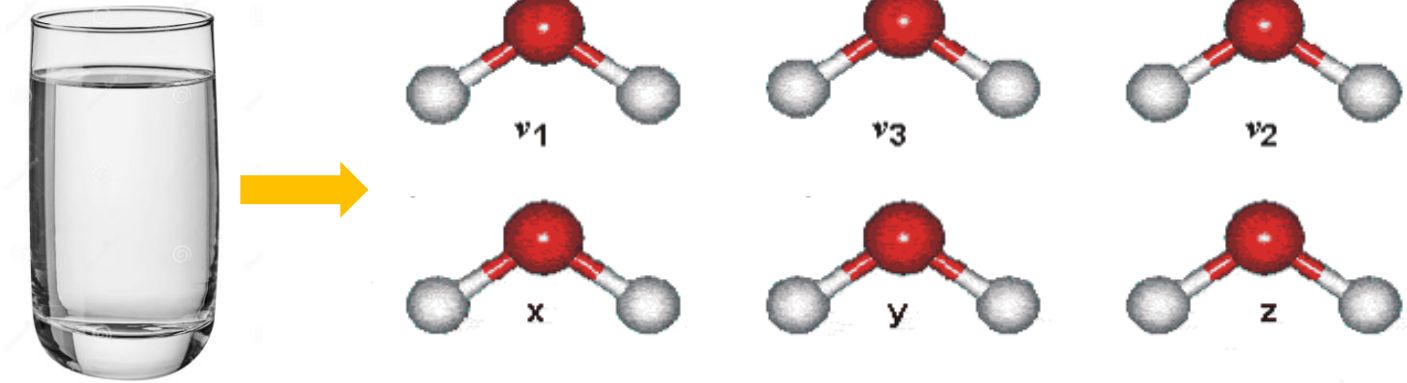

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Workshop “Dancing with molecules”

What can we learn from dancing?

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Hawaii

Japan

Portugal

What can we learn from dancing?

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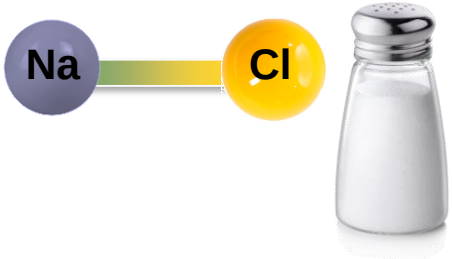
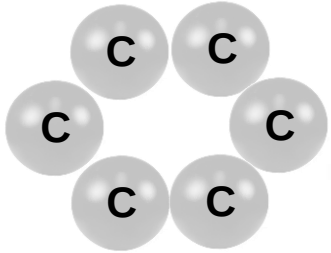
Breakdance

Valcer



Tango



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Workshop “Dancing with molecules”

What is Raman spectroscopy?

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Type	Mo	Cu
Bonding	Zn-S	Zn-Se
Mass	Si	Se

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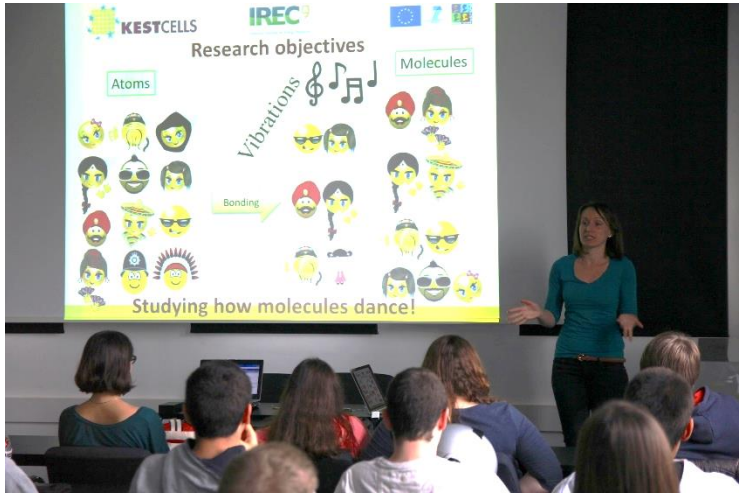
Workshop “Dancing with molecules”



(most) **Atoms (just like people) like to bond!**

Raman spectroscopy:
studying how molecules dance!

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Introduction

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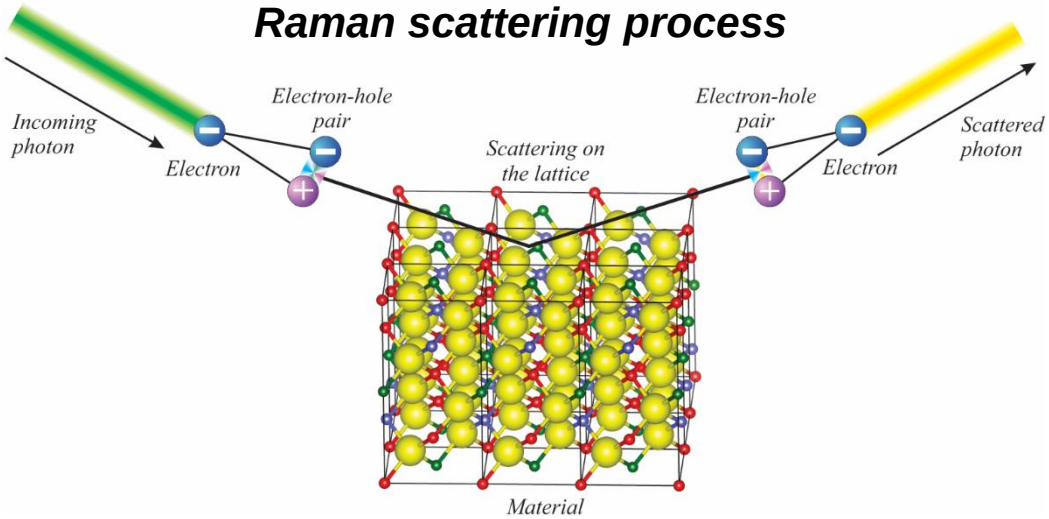
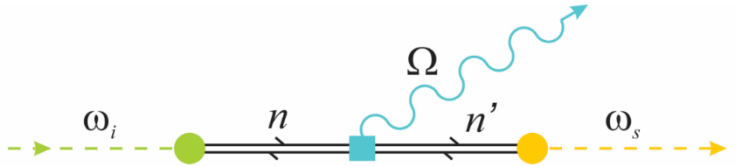
Raman instrument

Raman scattering process





Feynman's diagram

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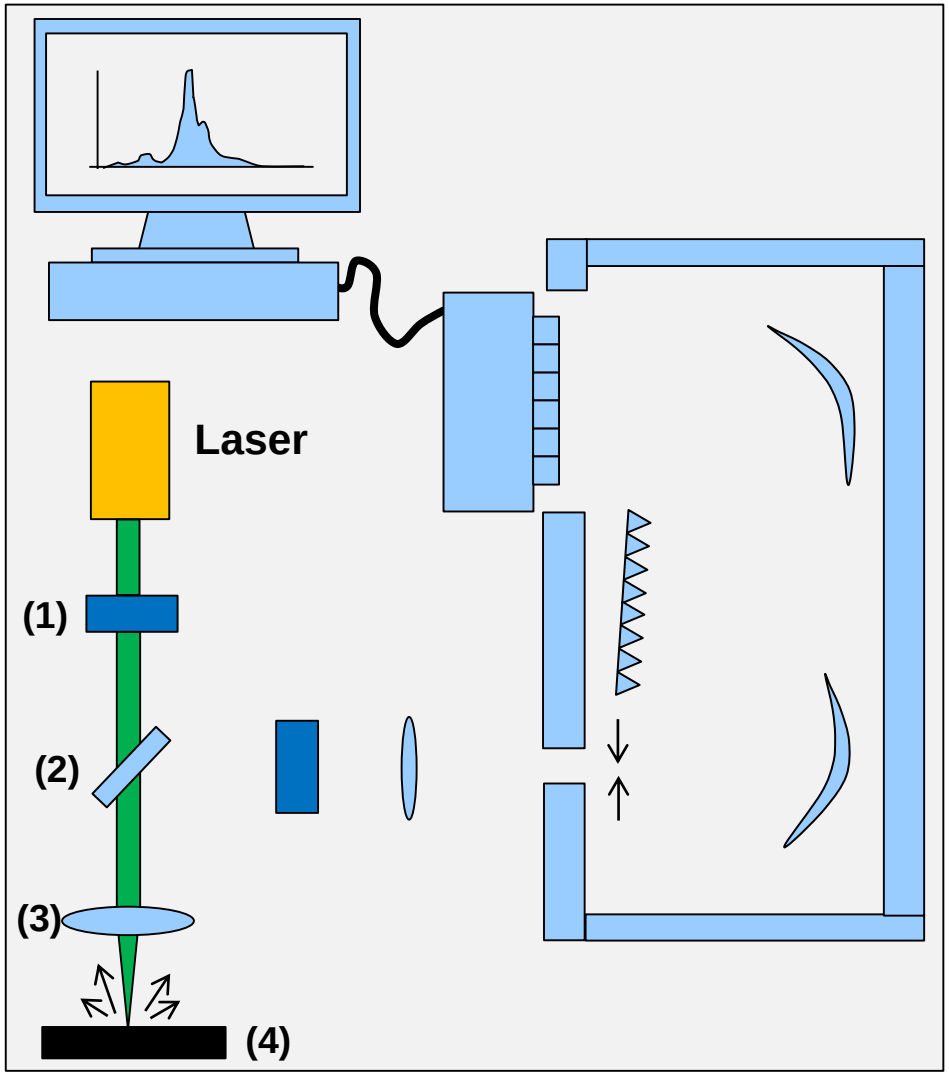
Raman spectroscopy system



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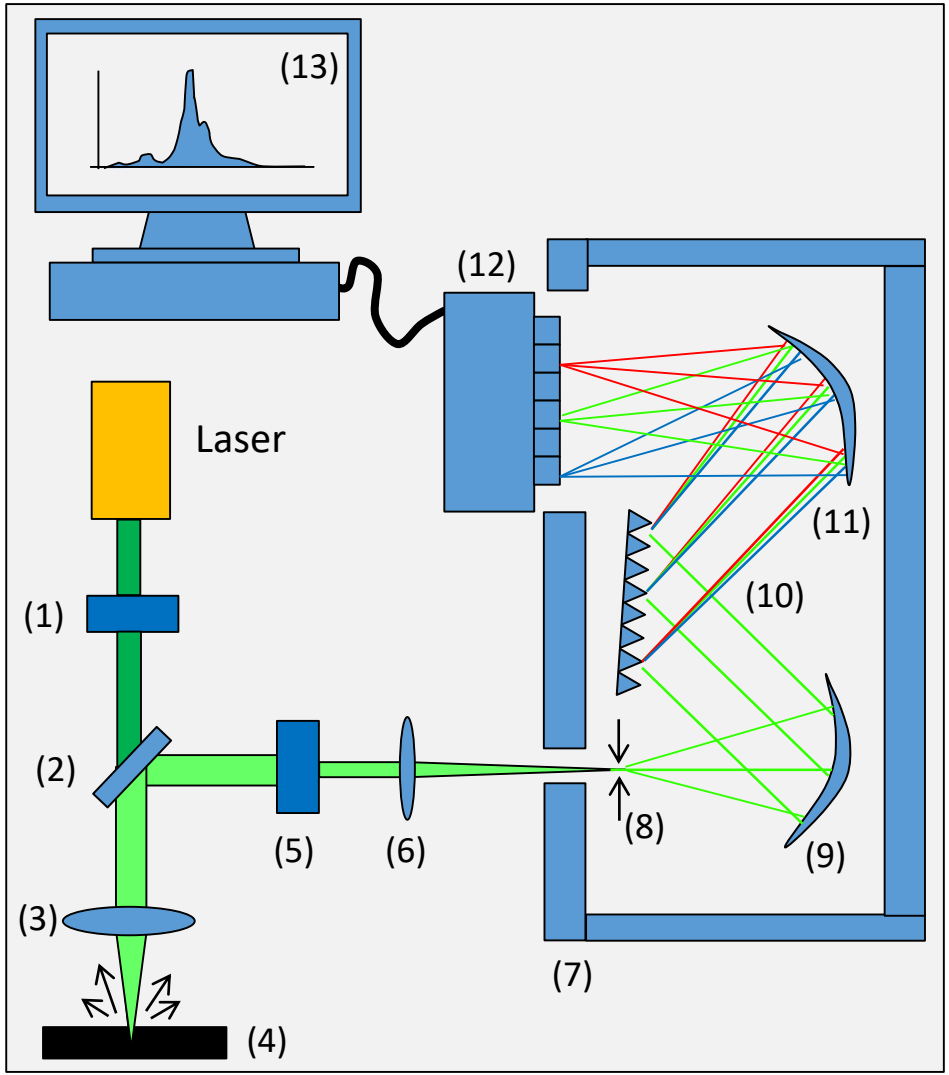
Raman spectroscopy system



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Introduction: Raman spectrum

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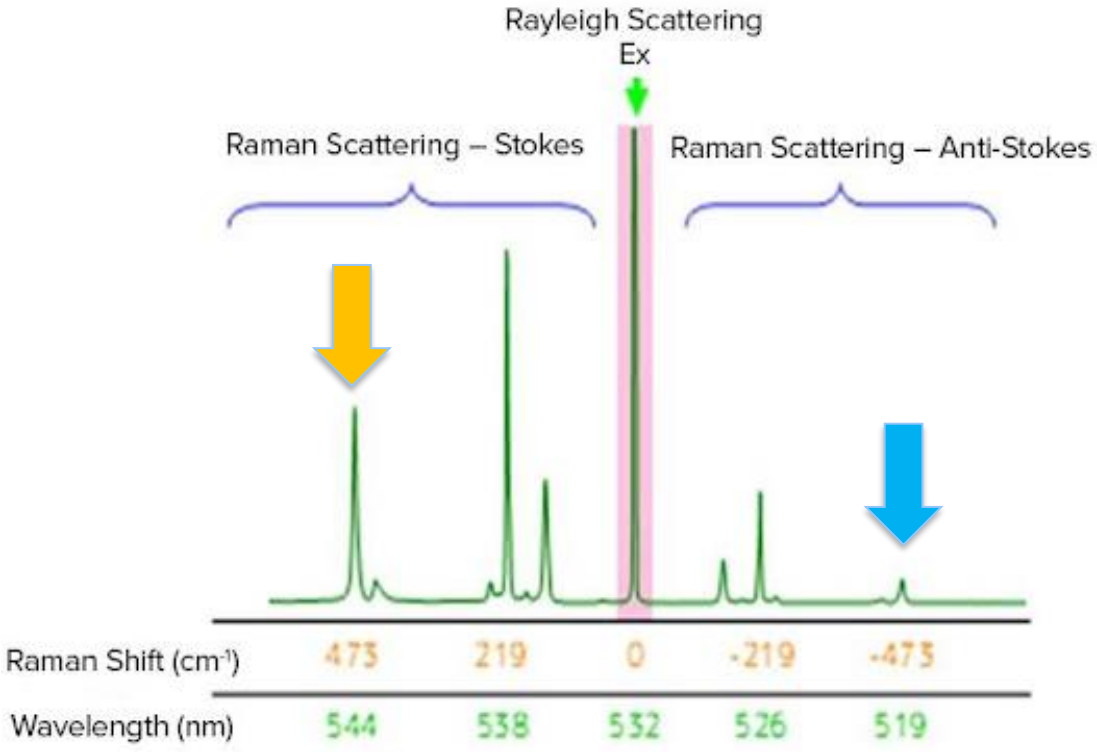

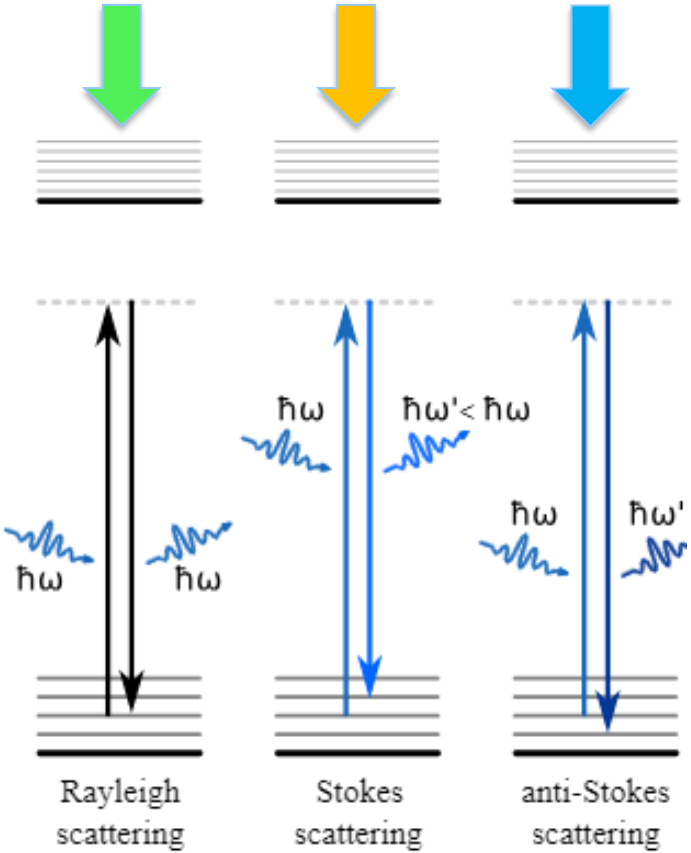

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Introduction: Raman spectrum

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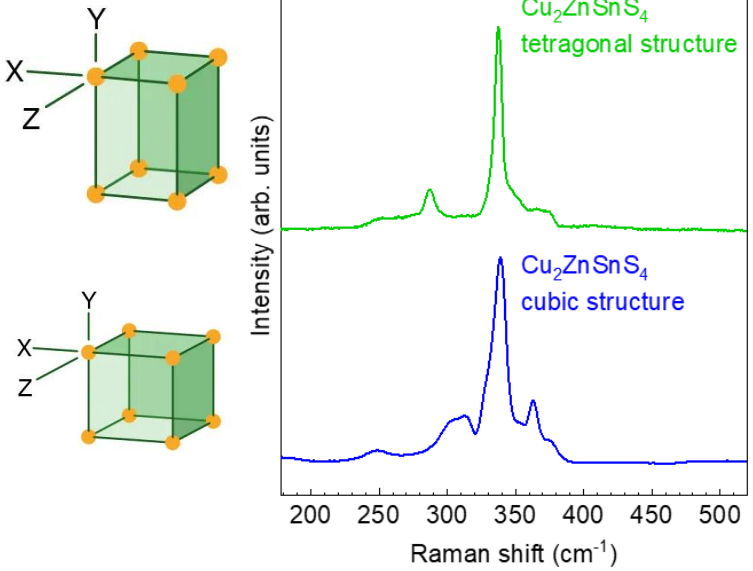
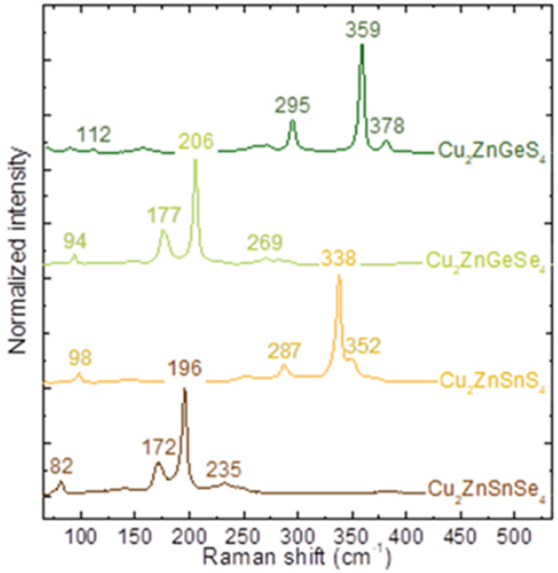
Raman spectrum provides indirect information about the energy of phonons created or annihilated in the scattering medium. Each spectrum is **a characteristic fingerprint** of the compound and contains information about:

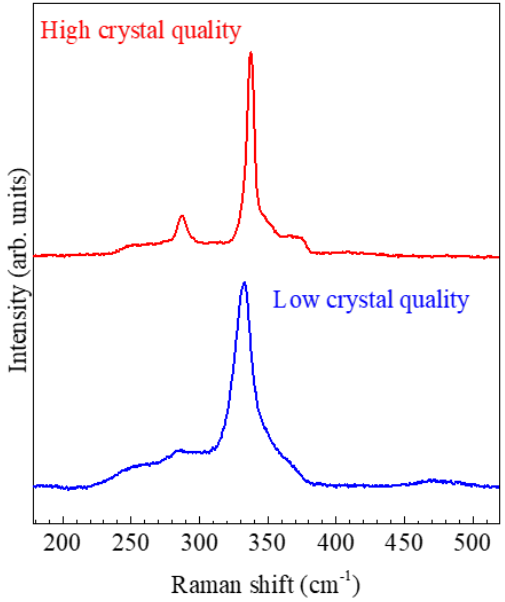
Crystal structure



Atomic Composition



Crystal quality



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Introduction: Raman spectroscopy

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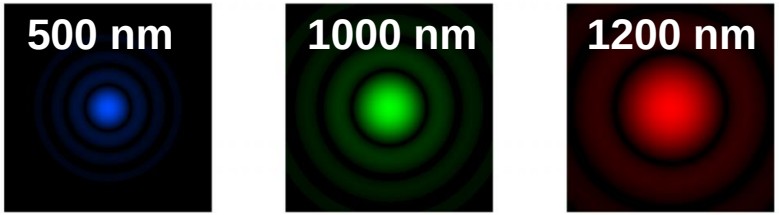
An ideal characterization tool for obtaining deeper insights about fundamental properties which is **simple** and **non-destructive**, offers **high resolution**, gives **structural and chemical information**, and is **applicable** at both **laboratory and mass-production scales**.

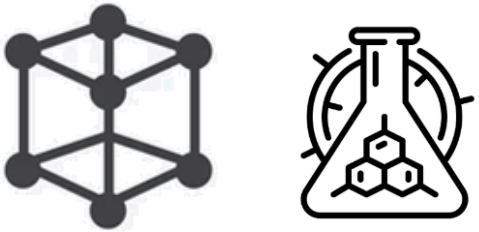
Non-destructive

High resolution (laser spot size)

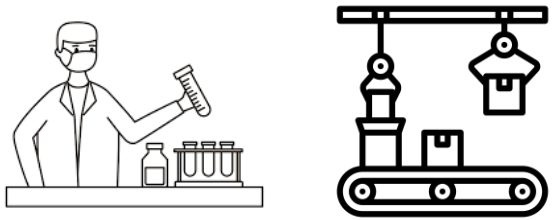


Fast

Structural and chemical information



Lab and industrial scales



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How to do measurements?

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Considerations to take into account when performing the measurements:

- ❑ **Excitation energy (laser wavelength)**
- ❑ **Power density and signal/noise ratio**
- ❑ **System alignment and calibration**

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Excitation energy (laser wavelength)

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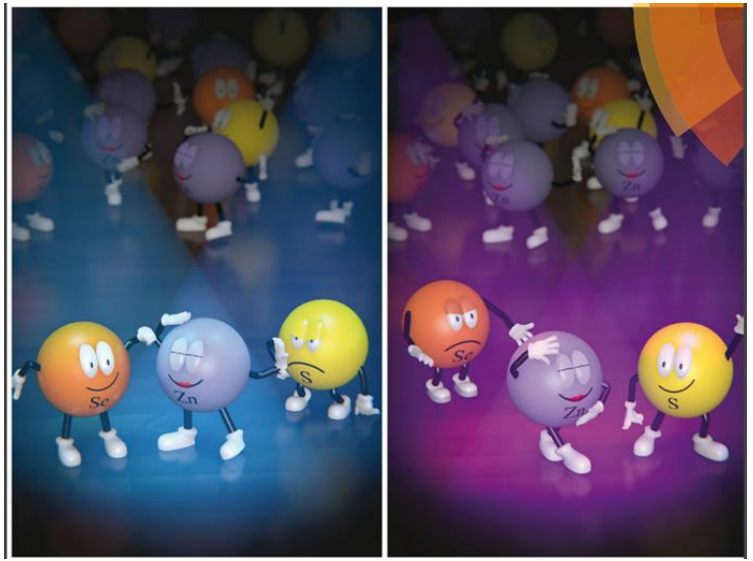
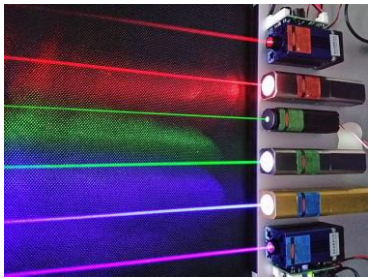
Music

Light



Laser wavelength =
Different types of music



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Excitation energy (laser wavelength)

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M. Dimitrievska, Phys. Chem. Chem. Phys., 2016,**18**, 7632-7640

Resonant Raman scattering of ZnS_xSe_{1-x} solid solutions: the role of S and Se electronic states

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Excitation energy (laser wavelength)

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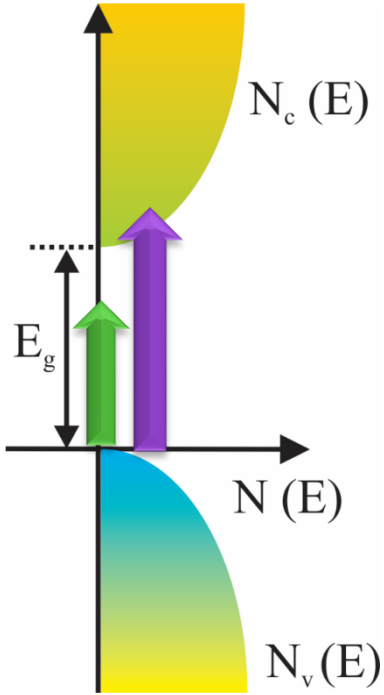
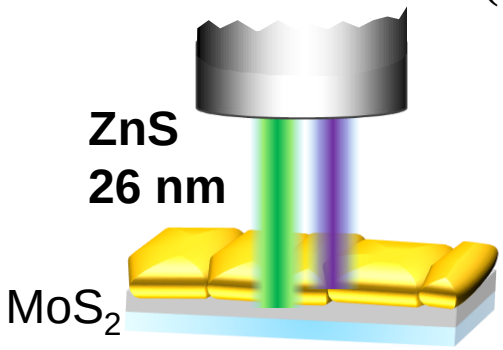
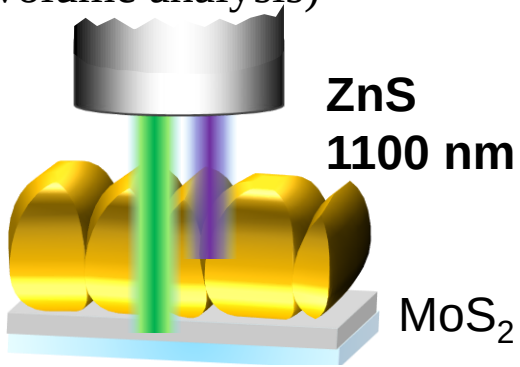
$\lambda_{ext} > E_g$: **strong** photon-matter interaction
(low penetration and small volume analysis)

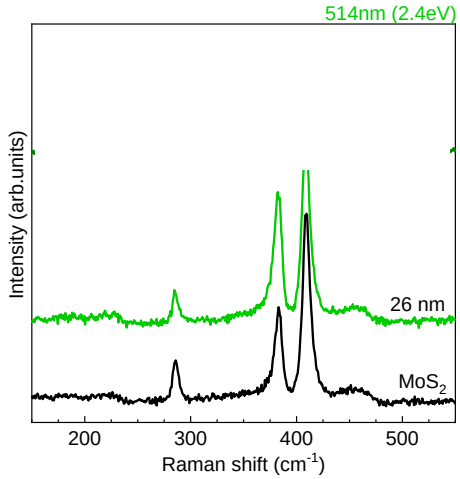
$\lambda_{ext} < E_g$: **weak** photon-matter interaction
(larger volume analysis)

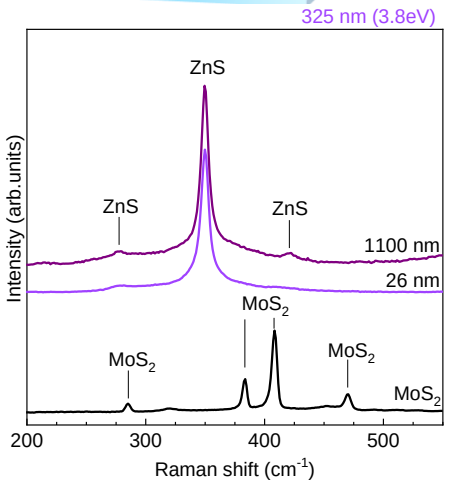
ZnS (E_g = 3.5 eV)











Multiwavelength excitation Raman spectroscopy

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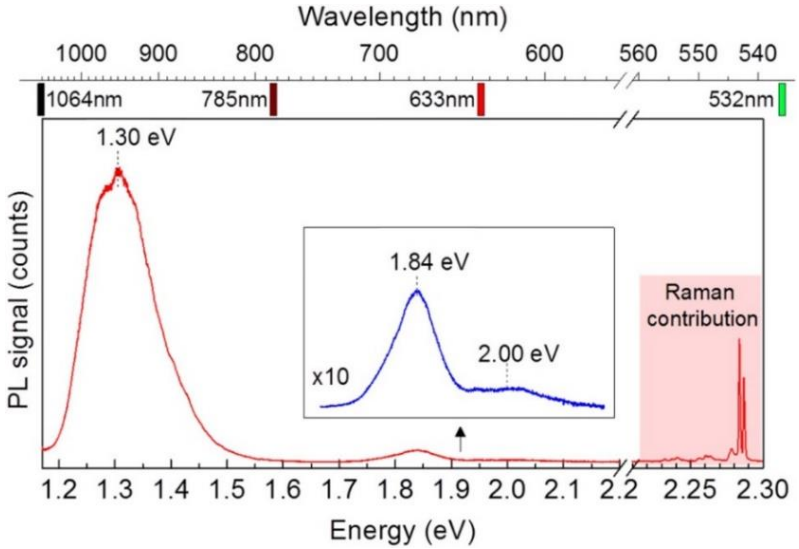
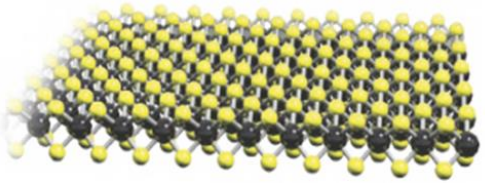
$\lambda_{ext} \approx E_g$ or E_i: **resonance conditions**

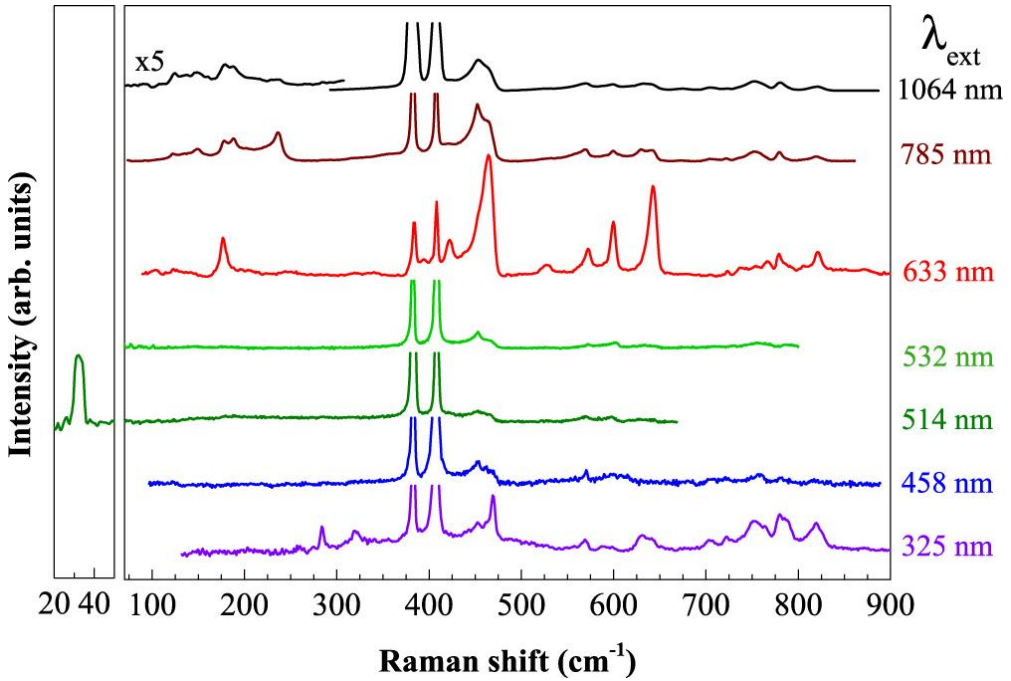
Raman intensity:

$$I \propto \frac{2\pi}{\hbar}\left|\frac{\langle 0|H_{e-r}|n\rangle\langle n|H_{e-Ph}|n'\rangle\langle n'|H_{e-r}|0\rangle}{(\hbar\omega_i-(E_{|n\rangle}-E_{|0\rangle})+i\Gamma)(\hbar\omega_s-(E_{|n'\rangle}-E_{|0\rangle})+i\Gamma)}\right|^2$$



MoS_2 (single crystal)





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M.Placidi, M. Dimitrievska et al. 2D Mater. 2 035006 (2015)

Multiwavelength excitation Raman spectroscopy: impurity identification

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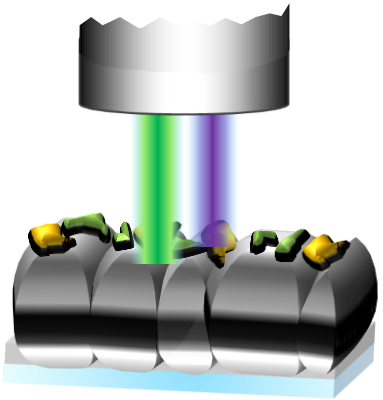
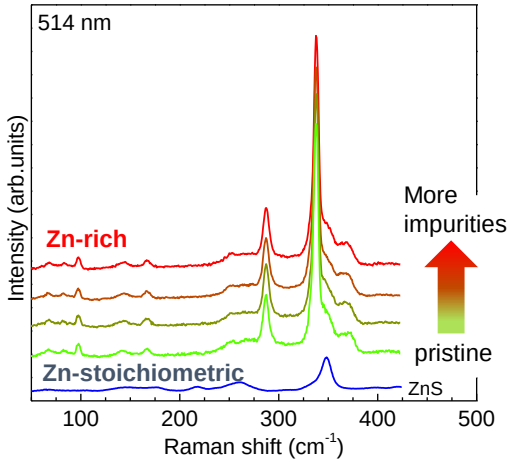
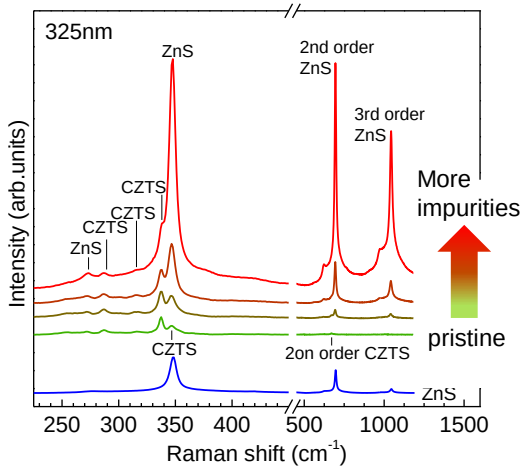
Assessment of ZnS in Cu_2ZnSnS_4



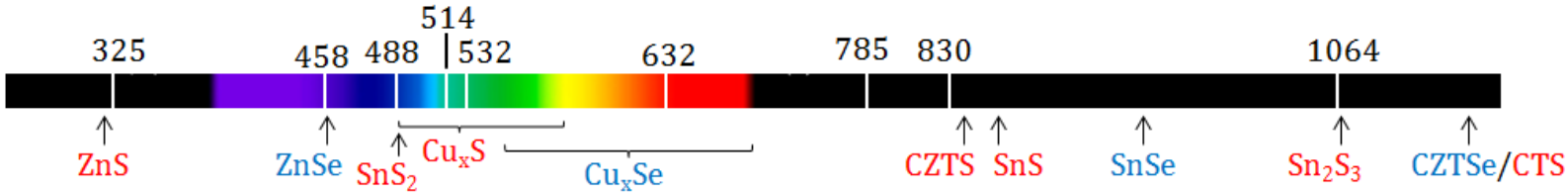
Standard Raman spectroscopy



Resonance Raman spectroscopy



Multiwavelength excitation Raman spectroscopy



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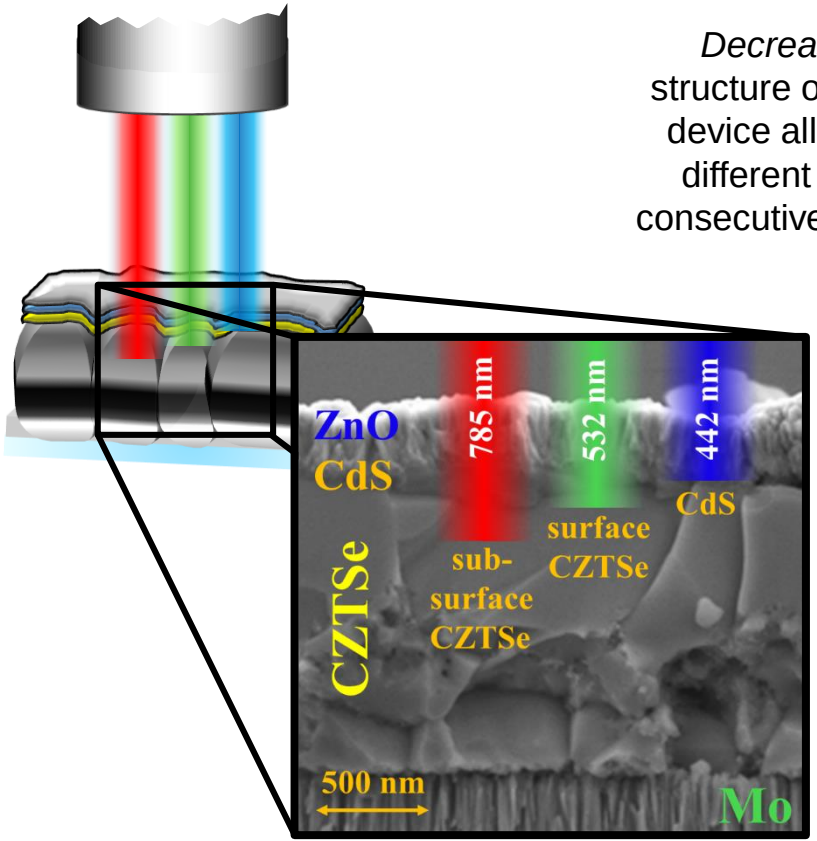
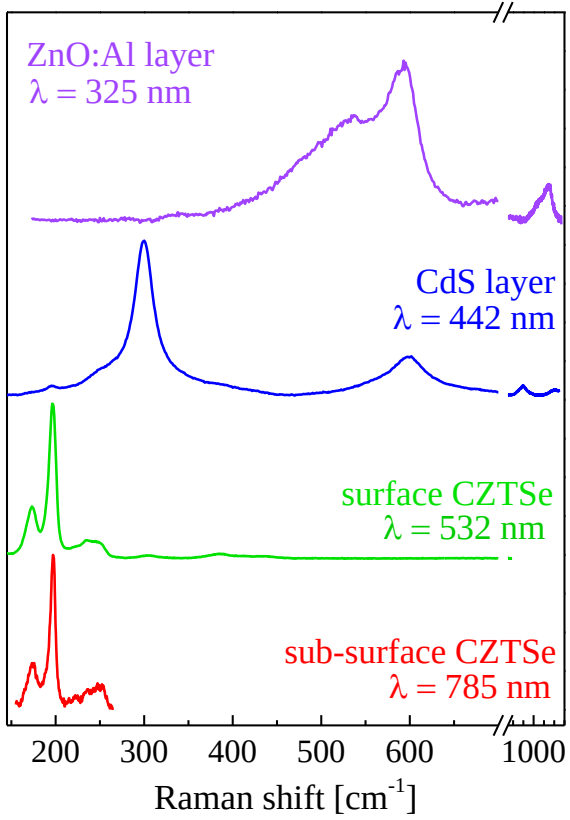
M. Dimitrievska et al. Sol. Energy Mater. Sol. Cells,149, 304–309 (2016)

Excitation energy: application

In-depth non-destructive characterization of layered devices



Decreasing band gap structure of the solar cell device allows *analyzing* different layers using a consecutive *lower energy excitation.*



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M. Dimitrievska et al. Sol. Energy Mater. Sol. Cells, 157, 462–467(2016)

Applied power density

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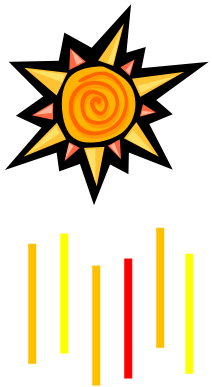
Raman spectroscopy is a **non-destructive technique**, but this is only **within certain limits**.

The irradiance of the sun is around 0.1W/cm^2.

If we focus a laser beam of **1 mW** through a microscope on a spot of **1 µm** diameter, then the obtained density of power is **5 orders of magnitude higher** than that of the Sun.

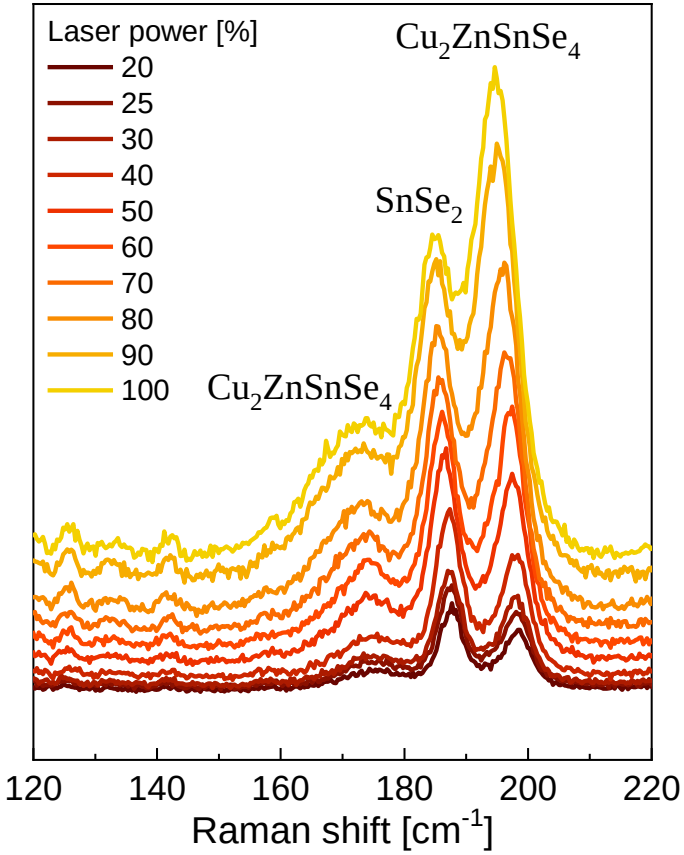


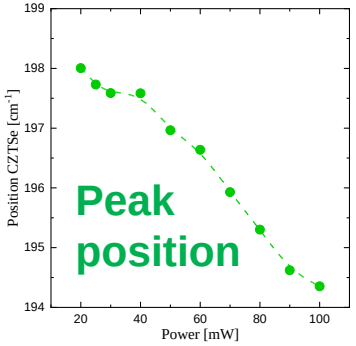
≈0.1W/cm^2

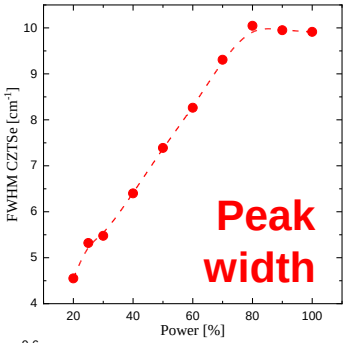
≈63600W/cm^2

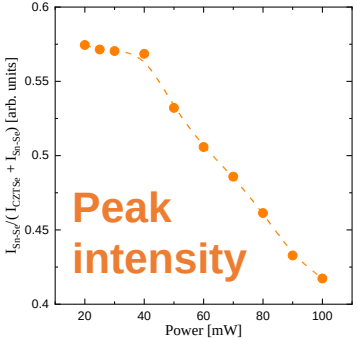
Applied power density

Power study

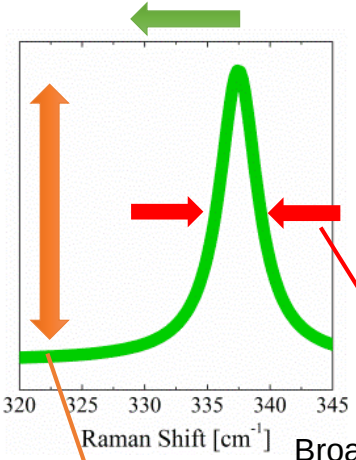








Peak position (due to the expansion of the lattice (**reversible**))



Broadening of peaks (due to the reduction of the phonon life time (**reversible**))

Change of the shape, intensity, or appearance of new peaks (due to recrystallization, decomposition or reaction between the phases (**irreversible**))

Applied power density

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Power study recipe

- Start with lowest power
- Measure Raman spectrum (1)
- Increase power for certain increment (don't change the measurement point)
- Measure Raman spectrum (2)
- Reduce power to minimum power
- Measure Raman spectrum (3)
- Compare (1) and (3) spectrum ← **Decision point**
- Increase power for certain increment (don't change the measurement point)
- Measure Raman spectrum (4)
- Compare (1) and (4) spectrum ← **Decision point**
- Increase power for certain increment (don't change the measurement point)
- Measure Raman spectrum (5)
- Compare (1) and (5) spectrum ← **Decision point**
- …..

Decision point: If you see differences between the spectra, go back to lower power, and do all measurements with that power. If no differences, increase power.

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Signal/noise ratio

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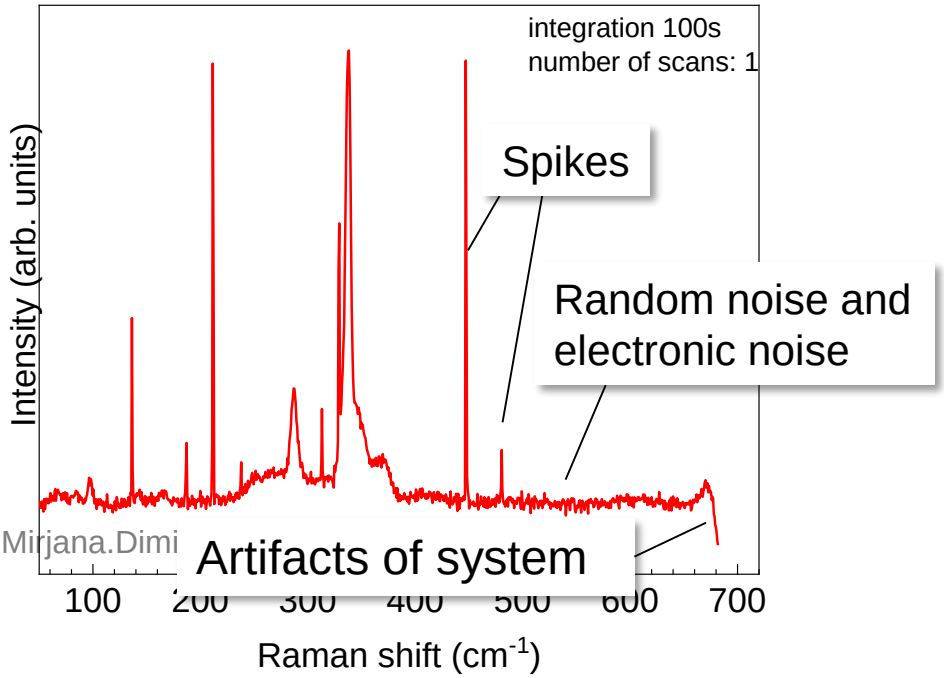
Low power density could induce small signal/noise ratio (SNR) that could make the interpretation of the Raman measurements more difficult.

There are **different types of noise**. Depending on their origin they can be reduced/solved or not.



Spike: originated from cosmic rays. The probability of occurrence increases with time acquisition

Random noise: intrinsic to measurement. It is reduced when the integration time is increased.

Electronic noise: intrinsic - depends on the detector. It limits the SNR of the system.

Artifacts of the system: intrinsic – depends of the optical system. It doesn't change with the integration time.

Signal/noise ratio

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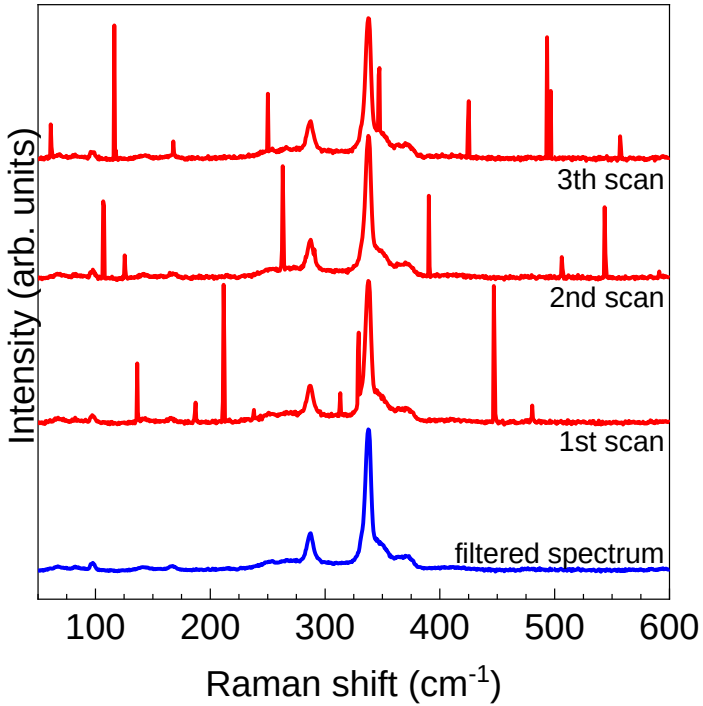
Different strategies could be utilized for the reduction of these effects:

Spikes: elimination of spikes can be obtained comparing different scans and making the average spectra after cleaning up the spikes



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Signal/noise ratio

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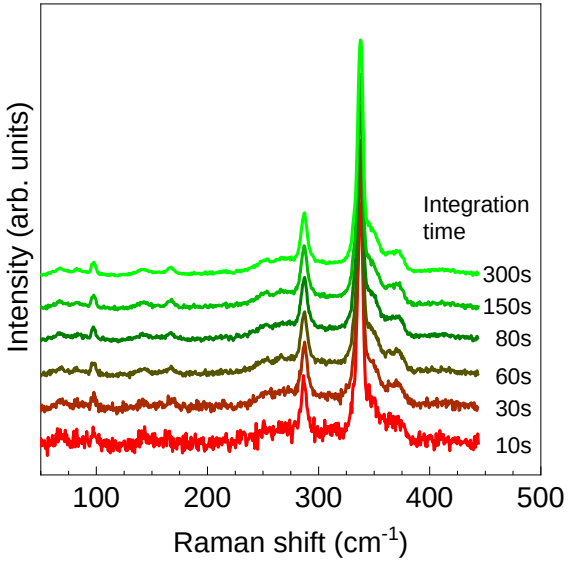
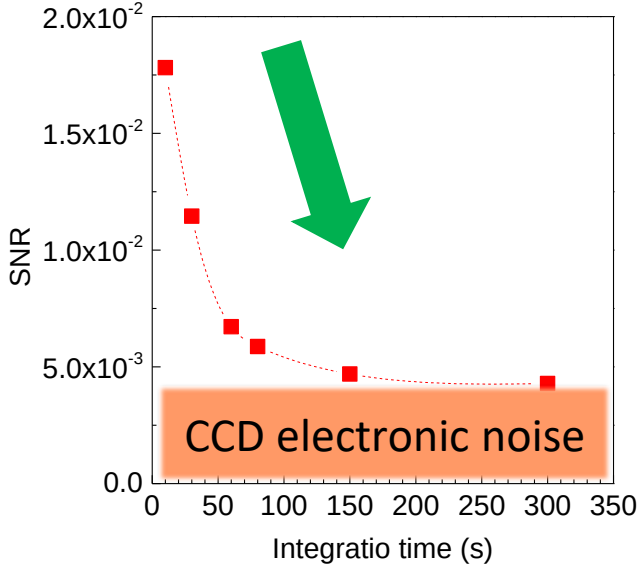
Different strategies could be utilized for the reduction of these effects:

Random noise: can be reduced by increasing the time of integration, however this will also cause the increase in the spike occurrence





However, **electronic noise** is intrinsic property of the detector. Using detectors with lower working temperature could reduce this effect.

In order to improve the signal/noise ratio, it is necessary to optimize the acquisition conditions, time integration and number of scans!

System alignment

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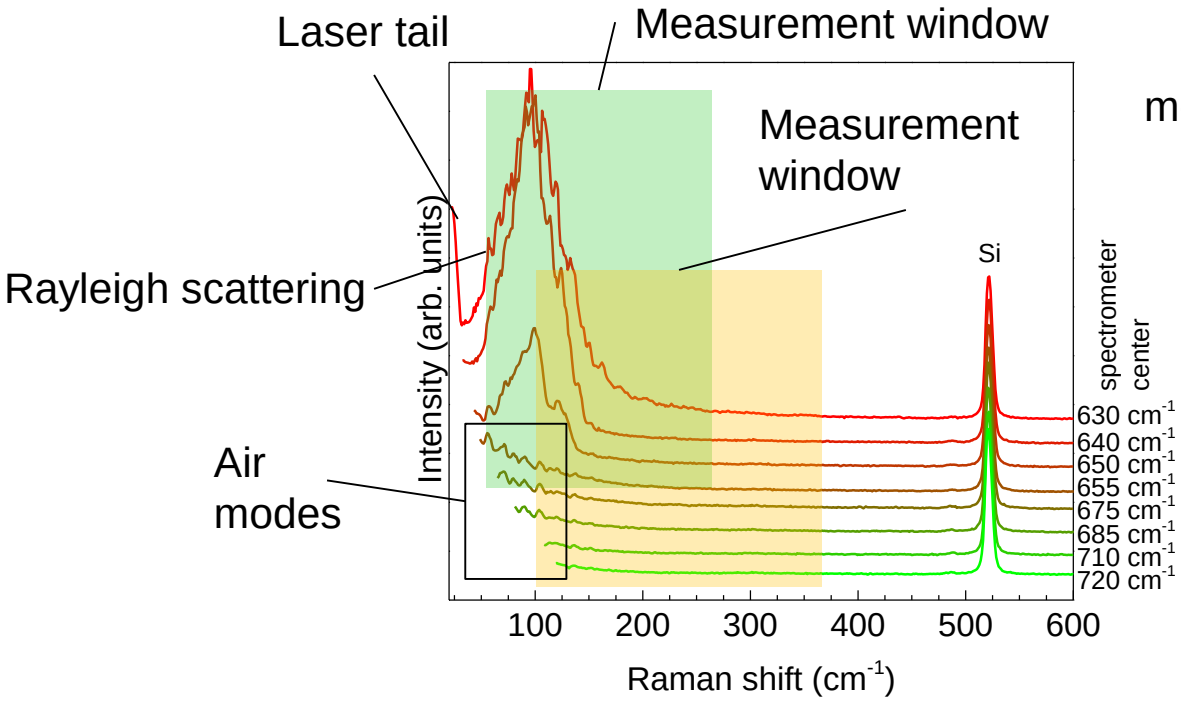
A correct alignment of the optical system is very important in order to optimize the signal/ noise ratio.



Example: Moving the measured spectral window

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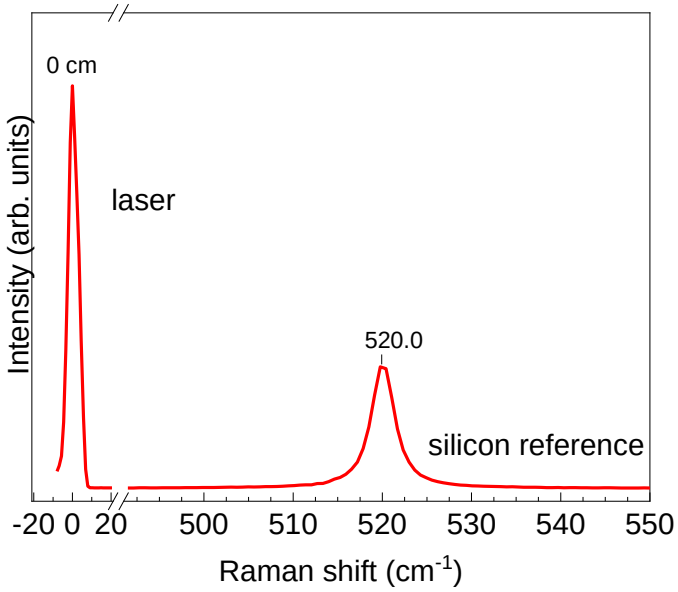
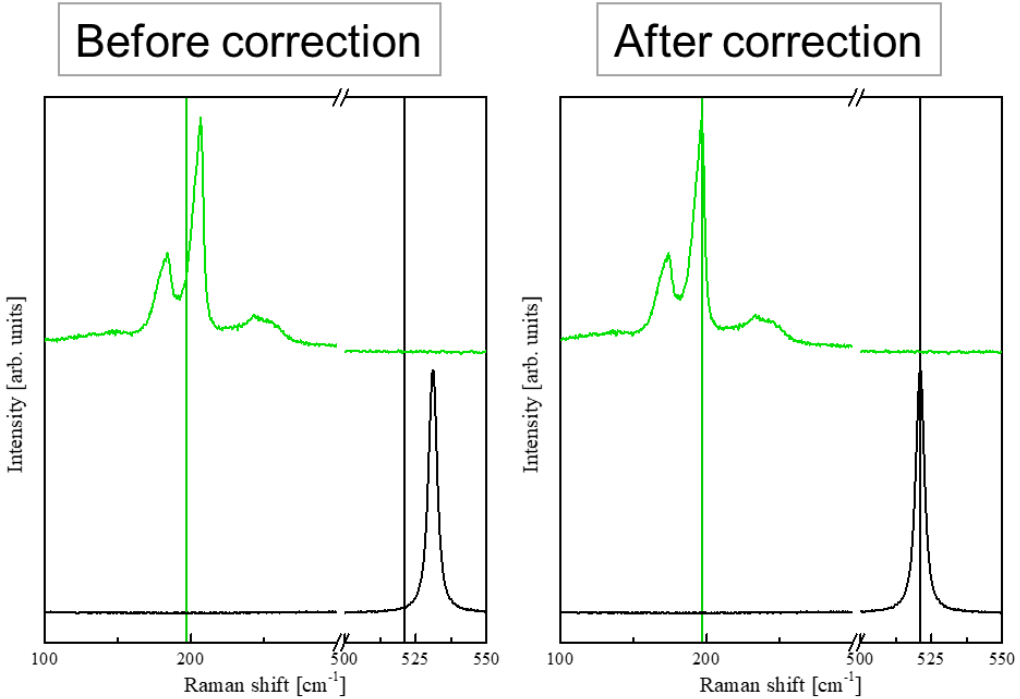
System alignment

Finally, a correct calibration of the Raman frequencies is required in order to obtain the correct positions of Raman peaks.

Correct calibration: it is necessary to define the laser position at 0 cm^{-1}. Also, it is necessary to use a reference sample in order to correct the calibration between pixels and wavenumbers. (For example, the silicon, peak position at 520 cm^{-1})





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How to do measurements?

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Recipe:

- **Pick the right energy excitation**
  - **Consider material's properties, such as band gap**
  - **What do you need to detect?**
  - **What do you want to investigate?**
- **Do a power study and optimize SNR**
  - **Choose the right power, integration time, and number of scans to obtain the lowest SNR, without damaging the material**
- **Choose the right spectral window for your study**
- **Measure reference samples for calibration of position as often as possible**

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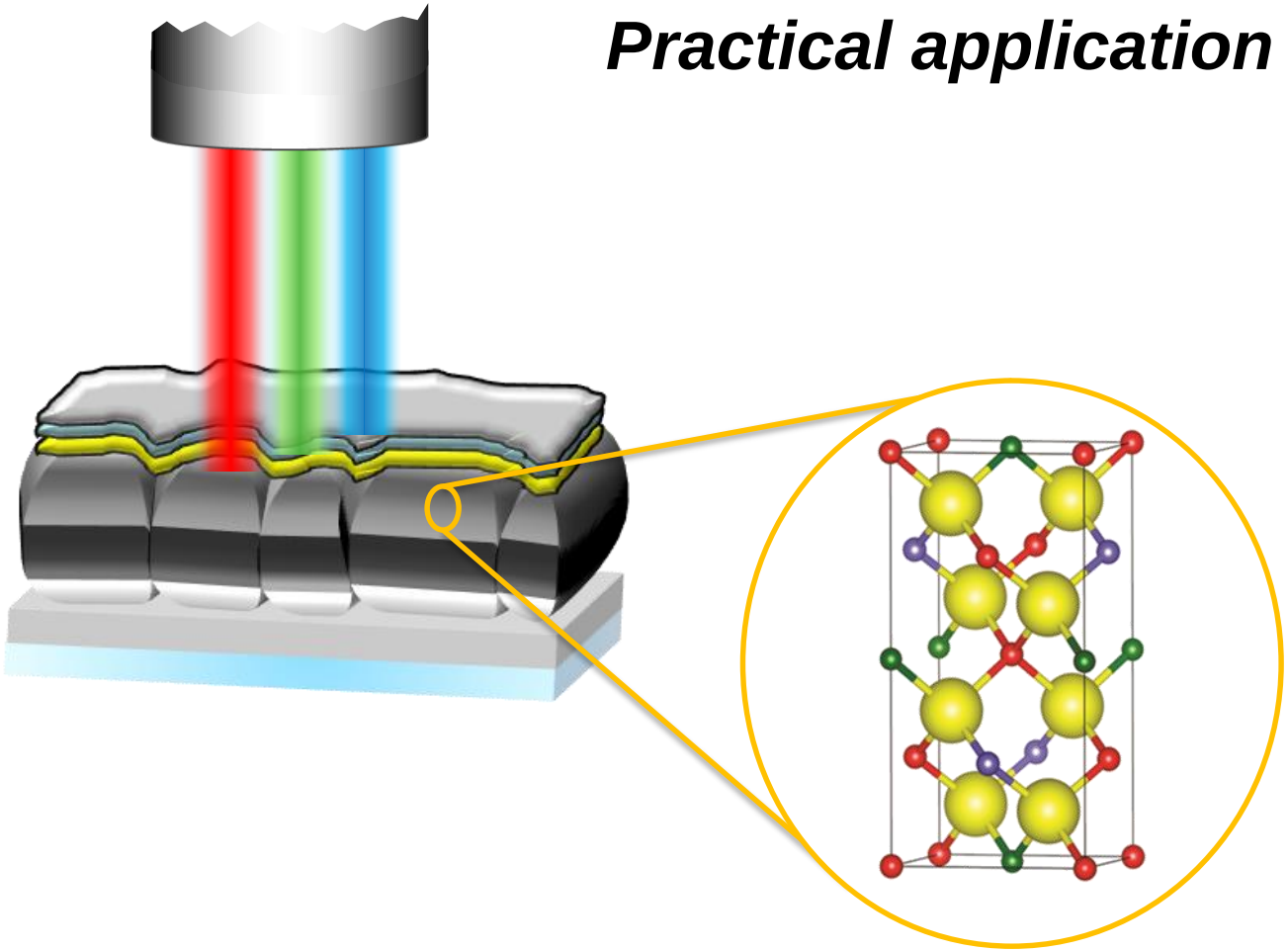
Practical application



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Application: Identification of fundamental modes

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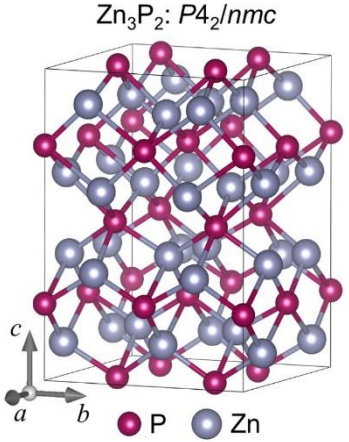
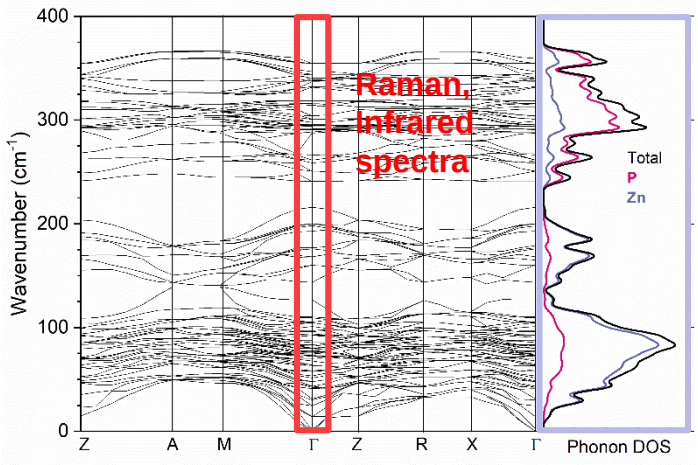
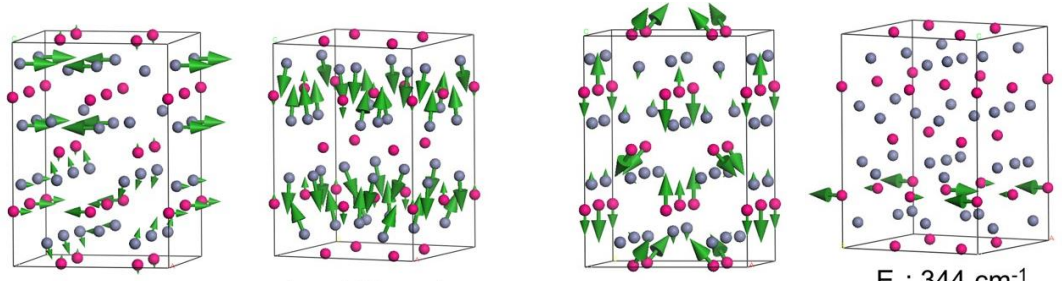
Lattice dynamic and structural characterization (DFT and experiment)



Phonon Dispersion and Density of States



Neutron vibrational spectra



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Application: Identification of fundamental modes

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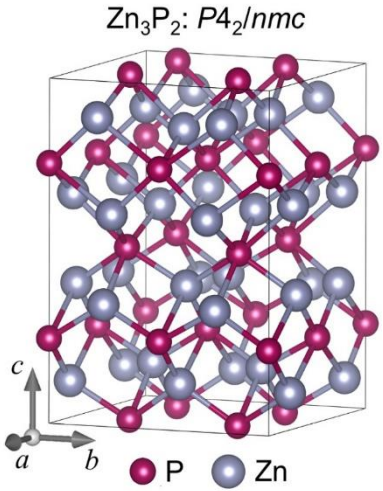
Identification of Raman mode positions and symmetry type



Irreducible representation for Raman active modes:

$$\Gamma_{Raman} = 9\mathrm{A}_{1g} + 10\mathrm{B}_{1g} + 4\mathrm{B}_{2g} + 16\mathrm{E}_{g}$$

Labels:

(A, B), E, T : non-, double-, triple- degenerate

A or B : symmetric or asymmetric with respect to the principal symmetry axis C_n

1 or 2 : symmetric or asymmetric with respect to the rotation around a two-fold axis (C_2) normal to the principal symmetry axis C_n

g or u : symmetric or anti-symmetric with respect to the inversion.

$$\mathfrak{R}_{\mathrm{A}_{1g}} = \begin{pmatrix} a & 0 & 0 \\ 0 & a & 0 \\ 0 & 0 & b \end{pmatrix}$$

$$\mathfrak{R}_{\mathrm{B}_{1g}} = \begin{pmatrix} c & 0 & 0 \\ 0 & -c & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$\mathfrak{R}_{\mathrm{B}_{2g}} = \begin{pmatrix} 0 & d & 0 \\ d & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$\mathfrak{R}_{\mathrm{E}_{g}} = \begin{pmatrix} 0 & 0 & e \\ 0 & 0 & e \\ e & e & 0 \end{pmatrix}$$

Irreducible representations:
https://www.cryst.ehu.es/#pointop

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Application: Identification of fundamental modes

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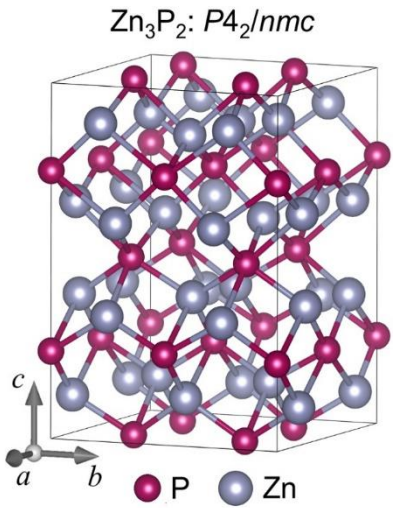
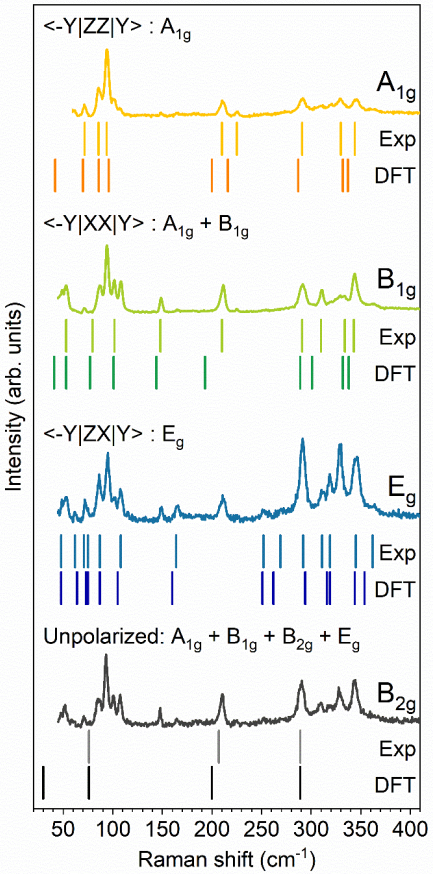
Symmetry of modes: polarization measurements



$$I \propto \left| v_i \, \Re_{xyz} \, v_s \right|^2$$

$$v_i = (\cos\theta \quad 0 \quad \sin\theta)$$

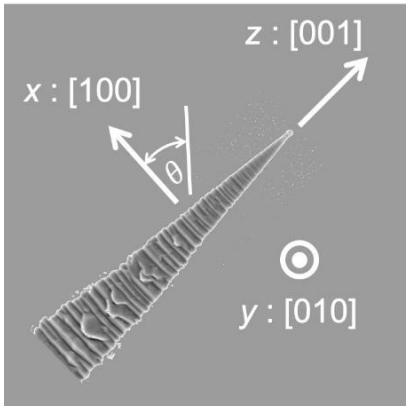
$$v_s^{\parallel} = \begin{pmatrix} \cos\theta \\ 0 \\ \sin\theta \end{pmatrix}; \; v_s^{\perp} = \begin{pmatrix} -\sin\theta \\ 0 \\ \cos\theta \end{pmatrix}$$

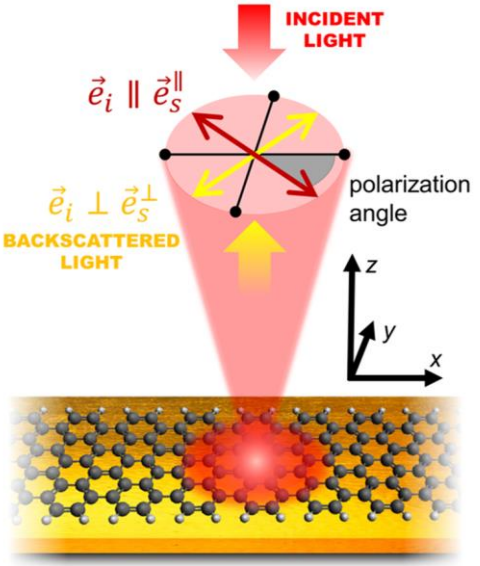


Proto notation

$$< -\mathrm{Y}|\mathrm{ZX}|\mathrm{Y} >$$

incoming radiation along *-y*-axis being polarized along *z*-axis with the backscattered (*y*) light polarized along *x*-axis





E.S. Stutz…M. Dimitrievska, Nanotechnology 32 085704 (2021)
M. Flor…M. Dimitrievska, Phys. Chem. Chem. Phys. 24 63 (2022)

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Application: Identification of fundamental modes

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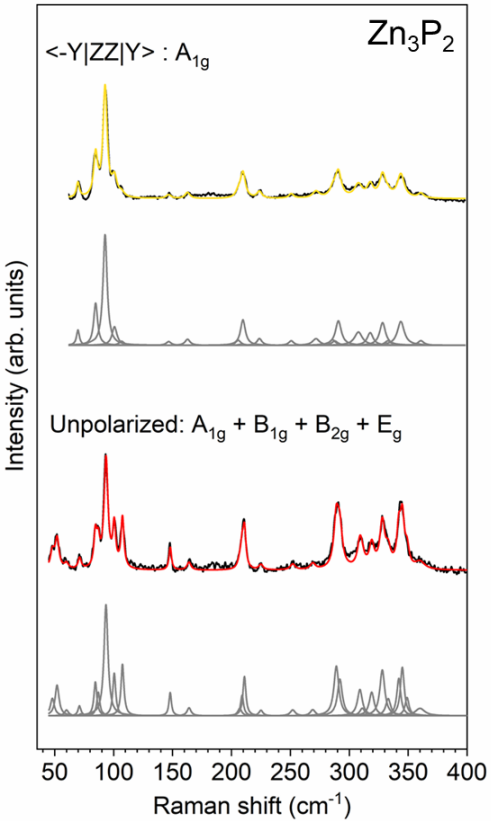
Identification of peak positions: deconvolution of Raman spectra



Procedure:

1) Determine which function is the most suitable for the investigated system (Lorentzian, Gaussian, Voight)
2) Baseline correction
3) Minimum number of meaningful peaks
4) Widths should have similar values for all peaks (fundamental one-phonon modes)
5) Peak positions should not change for different measurement configurations
6) Peak intensity should be a free parameter

You need to know your system well!

E.S. Stutz…M. Dimitrievska, Nanotechnology 32 085704 (2021)
M. Flor…M. Dimitrievska, Phys. Chem. Chem. Phys. 24 63 (2022)

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Application: Identification of fundamental modes

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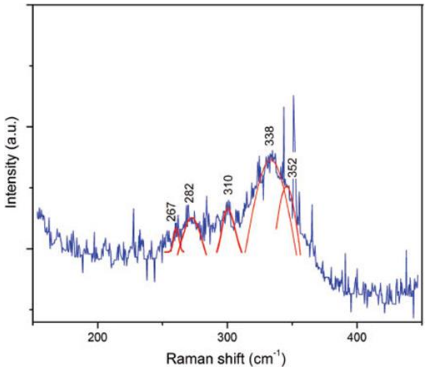
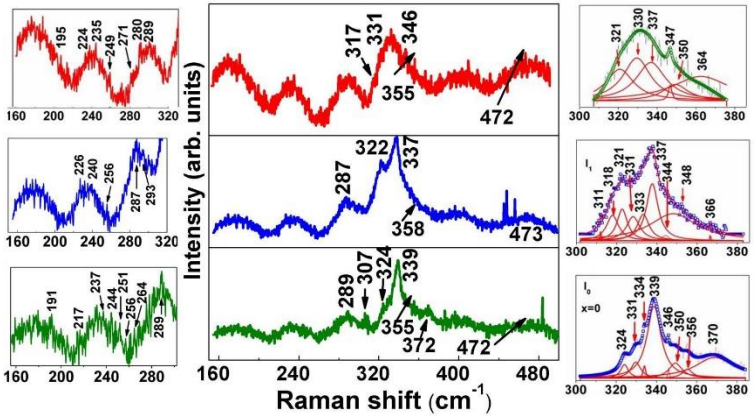
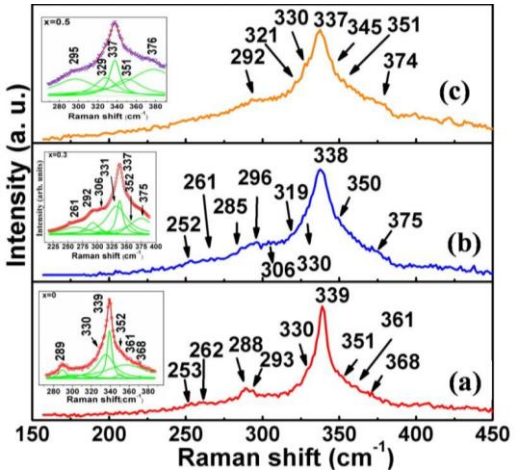
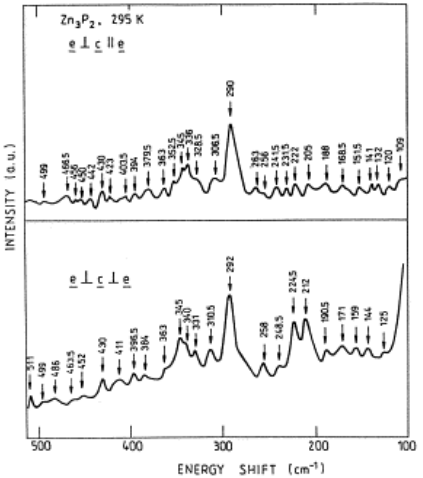
Identification of peak positions: bad examples









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Raman spectroscopy: defect identification

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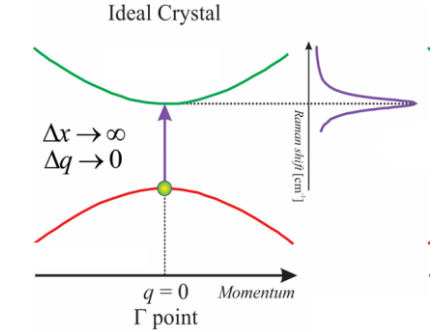
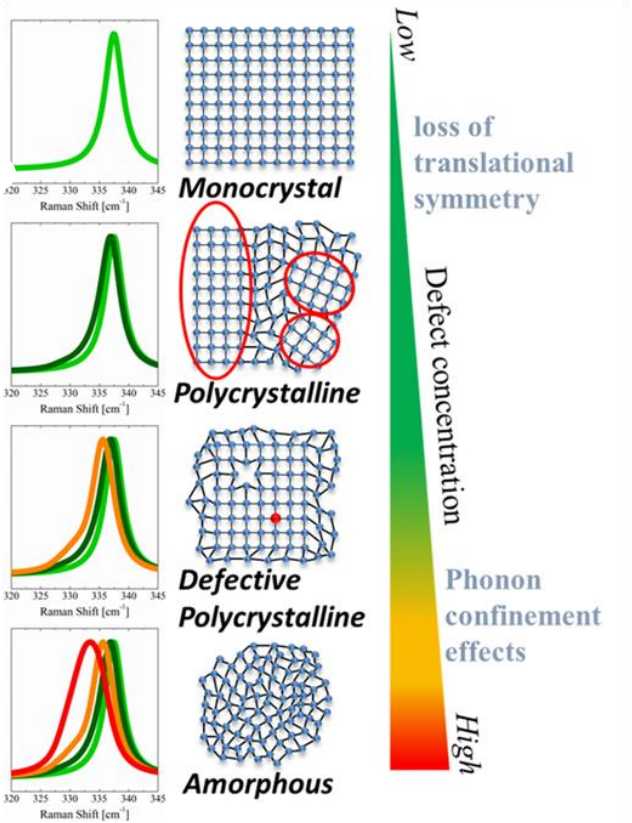
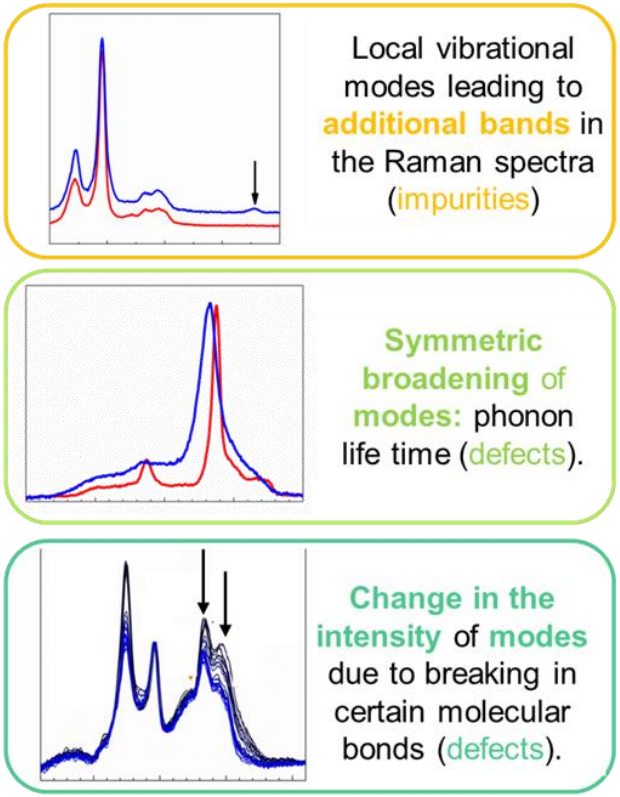


Raman features and defects



Effects of certain types of defects



M. Dimitrievska et al., Acta Materialia 70, 272–280 (2014)

M. Dimitrievska et al. Appl. Phys. Lett. 106, 073903 (2015)
M. Dimitrievska et al. J. Mater. Chem. A,7, 13293-13304 (2019)

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Application: Defects – Phonon confinement model

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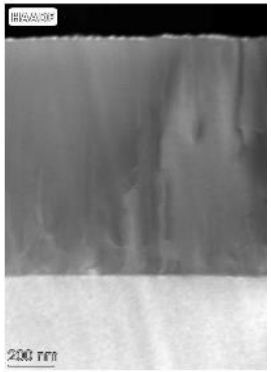
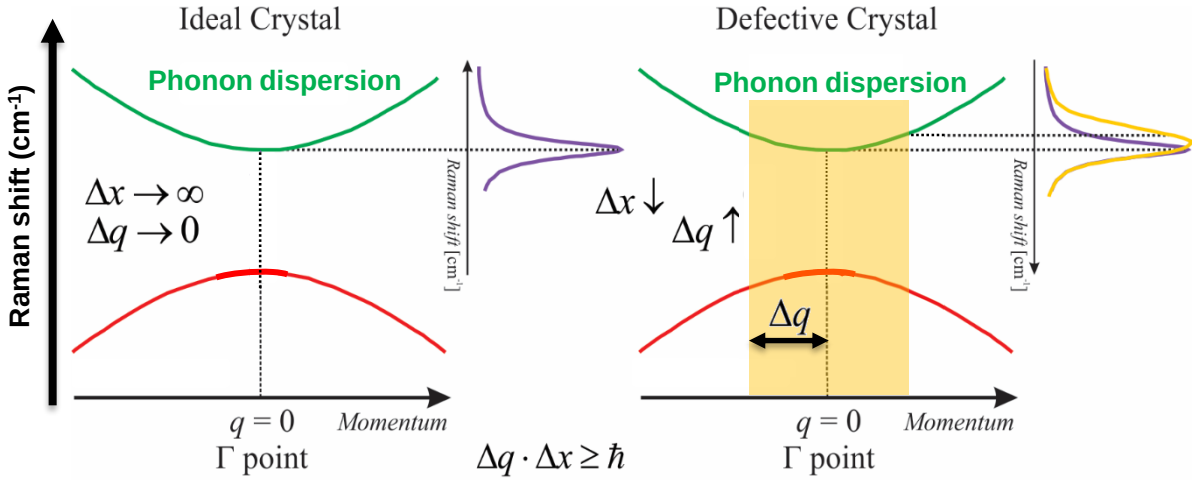
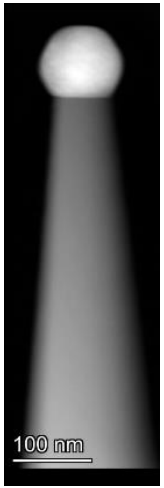
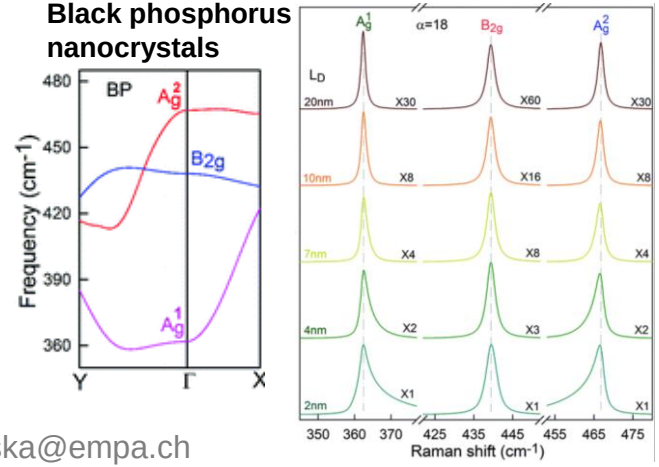






Black phosphorus nanocrystals



$$I(\omega) = \int_0^{\Gamma N} \frac{9\, j_1^2\left(L\,q/2\right)/\left(L\,q/2\right)^2}{\left[\omega - \left(\omega(q) + \Delta\omega_c + \Delta\omega_s\right)\right]^2 + \frac{\Gamma^2}{4}} 4\pi\, q^2\, \mathrm{d}q$$

Correlation length (L)
Crystal quality estimation model

M. Dimitrievska et al., Acta Materialia 70, 272–280 (2014)
T. Lin Nanoscale, 10, 8704-8711 (2018)

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Application: Defect cluster identification

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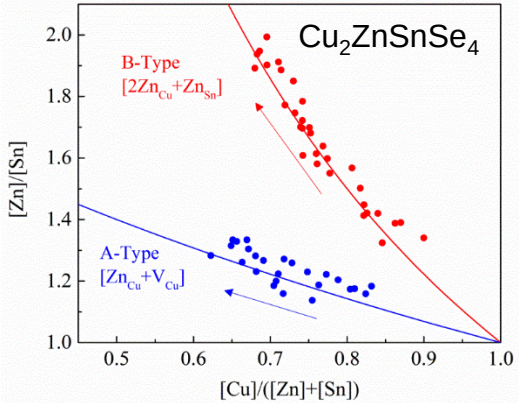
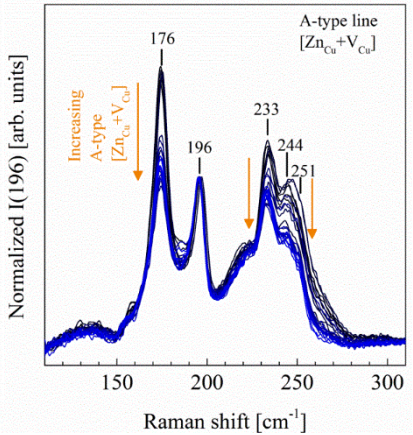
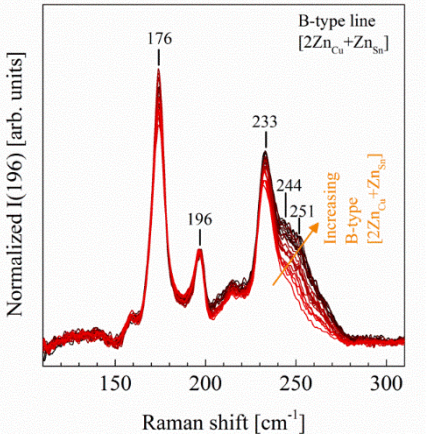
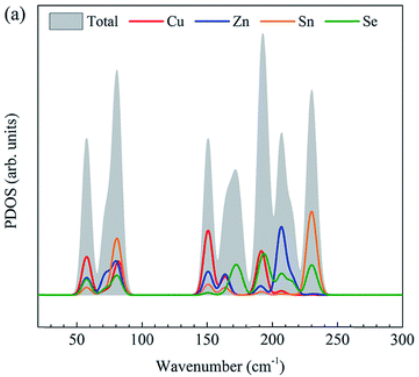
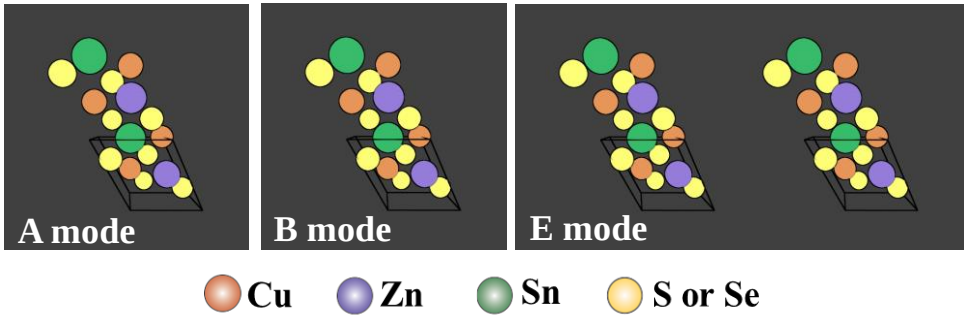
Combinatorial studies and DFT calculations:
simple methodology for identifying defects in $Cu_2ZnSnSe_4$.











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M. Dimitrievska et al. J. Mater. Chem. A, 7, 13293-13304 (2019)

Application: Compositional assessment

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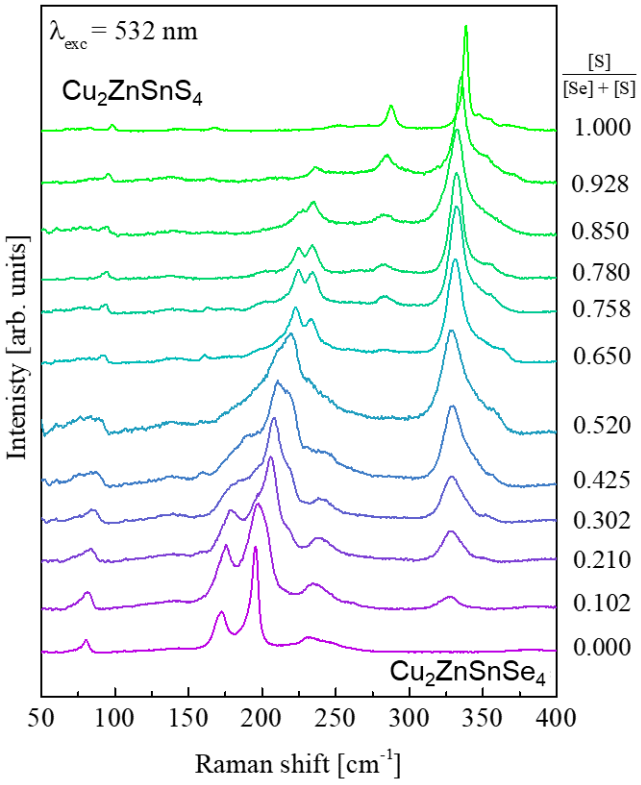
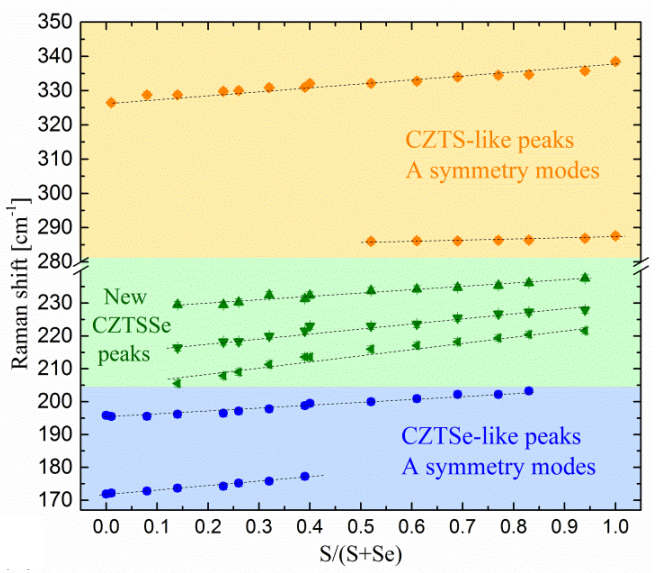
The shape of Raman spectra is very sensitive to changes in composition.



Building methodologies for compositional assessment:

1) Based on peak positions
2) Based on intensity ratio between certain modes



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M. Dimitrievska et al. J. Alloys Compd., 628, 464–470 (2015)

Application: Compositional assessment

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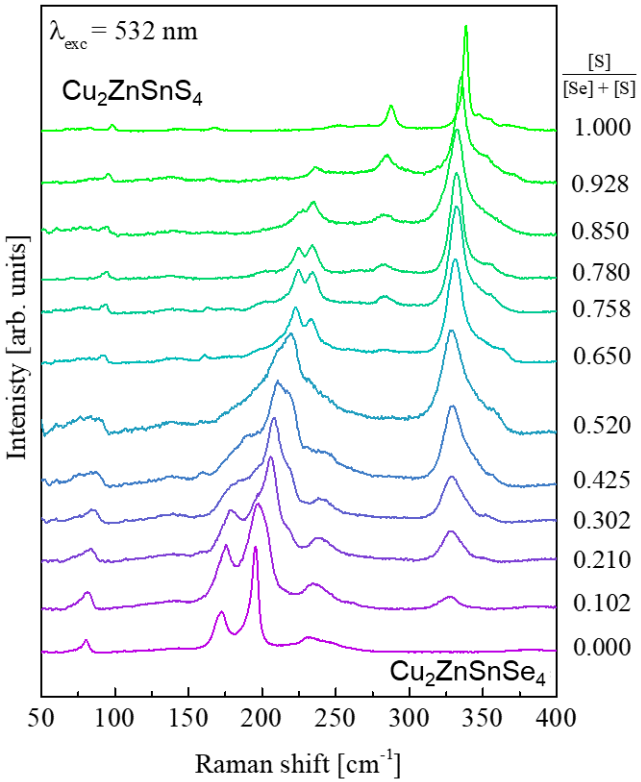

Building methodologies for compositional assessment:

1) **Based on peak positions**
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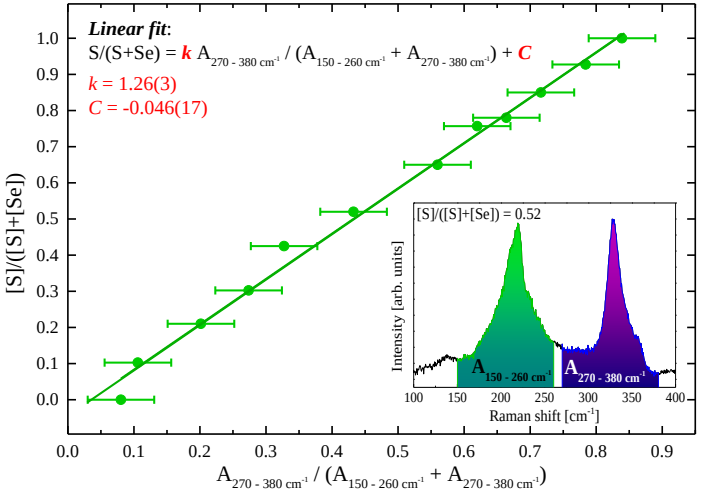

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M. Dimitrievska et al. J. Alloys Compd., 628, 464–470 (2015)

Conclusions

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- **Introduction: Raman spectroscopy**
- **Considerations to take into account when performing the measurements:**
  - **Excitation energy**
  - **Power density and signal/noise ratio**
  - **System alignment and calibration**
- **What can you do with Raman spectroscopy?**
  - **Fundamental identification of modes**
  - **Crystal quality / defect assessment**
  - **Compositional assessment**

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Literature

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- **Theory: M. Cardona: Fundamentals of Semiconductors (https://doi.org/10.1007/978-3-642-00710-1)**

- **Experiment: B. Schrader: Infrared and Raman Spectroscopy: Methods and Applications (https://doi.org/10.1002/9783527615438)**

- **Crystal and symmetry groups, irreducible representations, Raman active modes: Bilbao Crystallographic Server (https://www.cryst.ehu.es/)**

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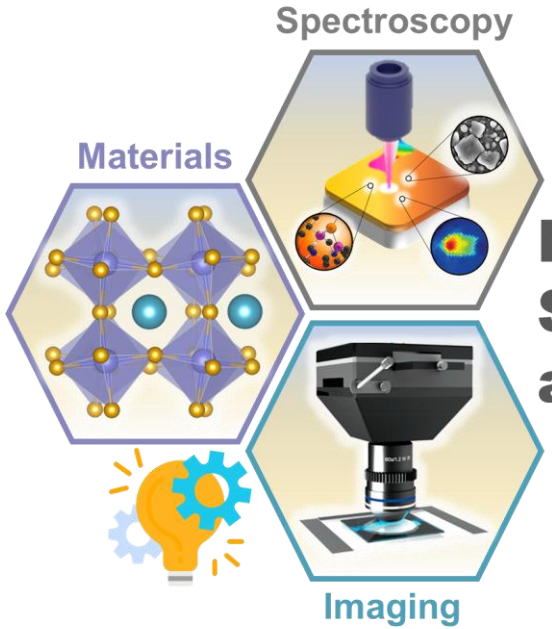
Thank you for your attention!



Nanomaterials Spectroscopy and Imaging

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Nanomaterials Spectroscopy and Imaging

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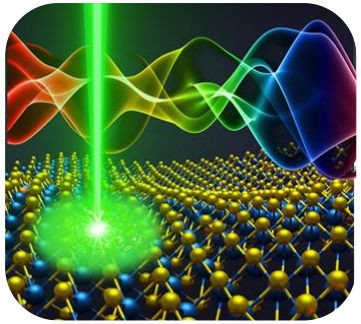

Raman spectroscopy at the nanoscale: from materials to devices

Mirjana Dimitrievska

Transport at Nanoscale Interfaces Laboratory

Swiss Federal Laboratories for Material Science and Technology (EMPA)

Switzerland

New materials discovery

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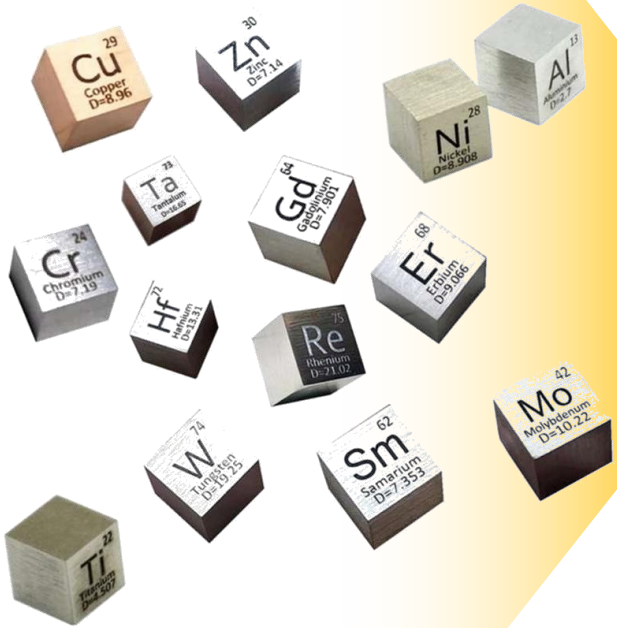
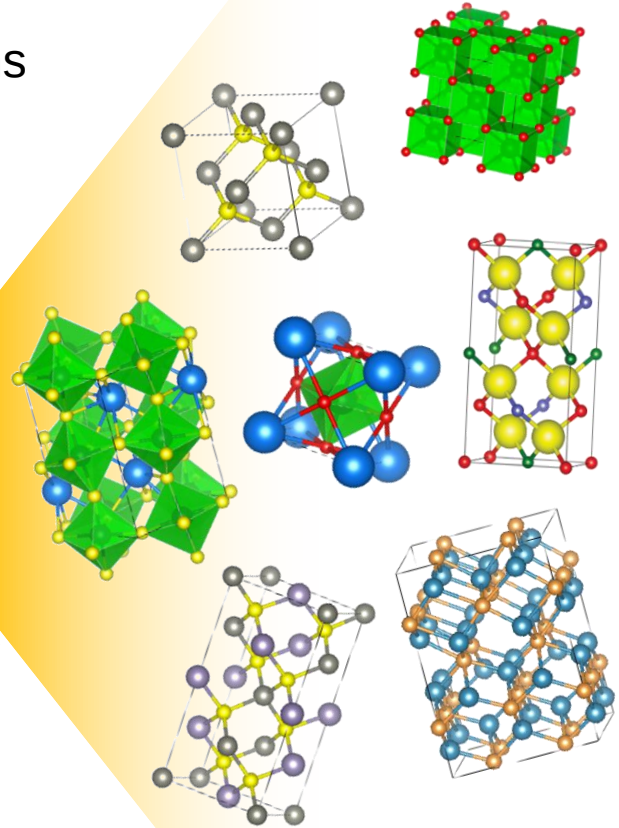
Advanced modeling/simulations
Machine learning





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Selection process of materials for applications

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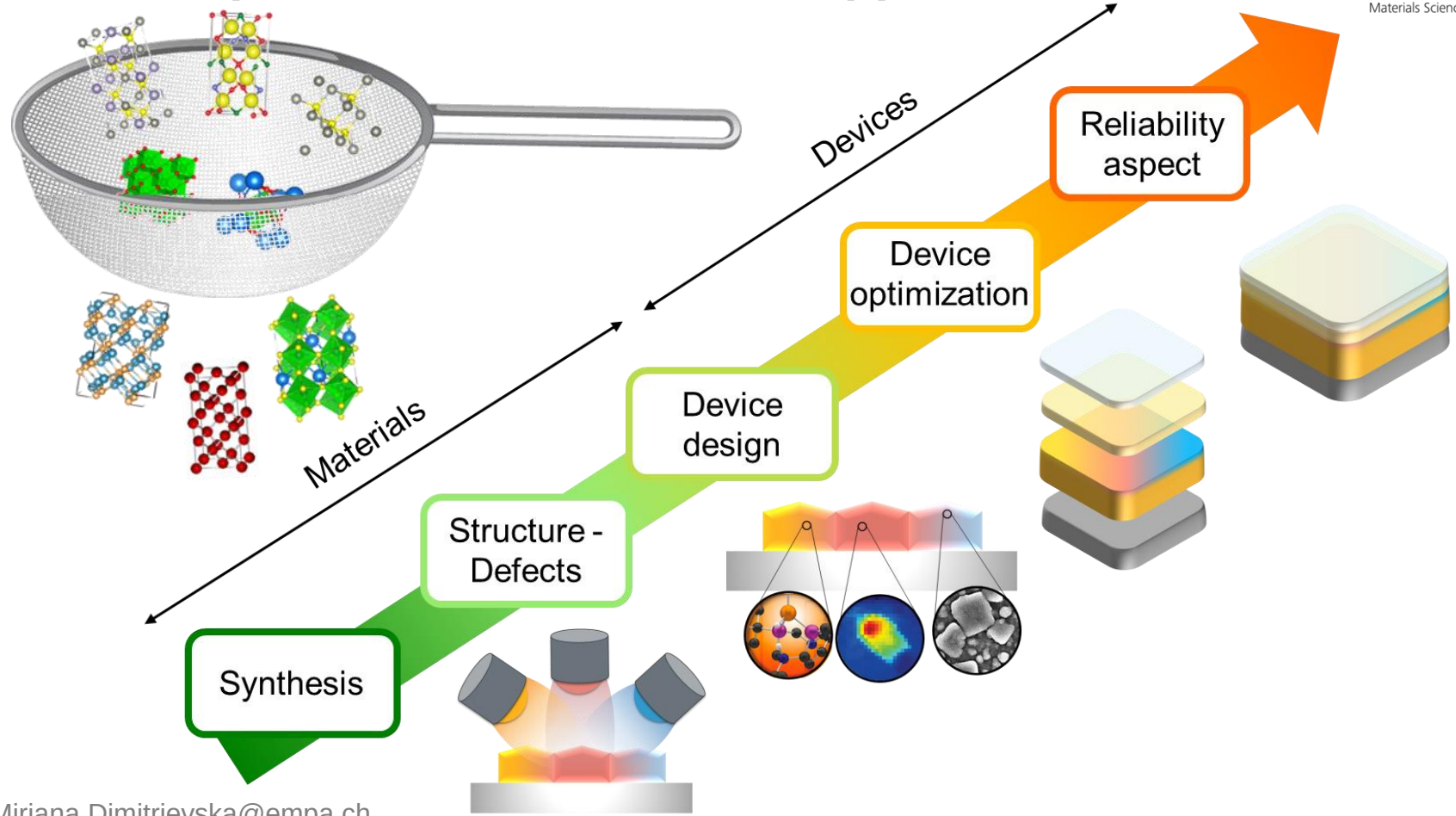

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Materials design roadmap: Raman perspective

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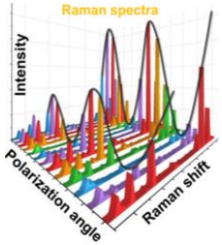
Reference Raman studies

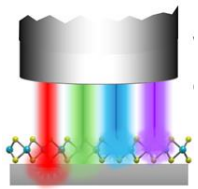
Applied Raman studies

X

Theory: Lattice dynamics calculations

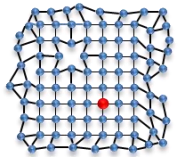


Experiment: Polarization Raman measurements

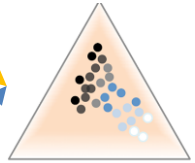


Experiment: Multiwavelength excitation Raman measurements

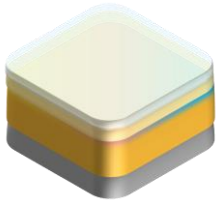
high crystal quality, stoichiometric samples



Defect identification



Secondary phase identification: phase diagram



Structure-function correlation: Device performance

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Materials design roadmap: Raman perspective

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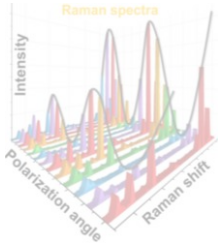
Reference Raman studies

Applied Raman studies

?

Theory: Lattice dynamics calculations



Experiment: Polarization Raman measurements

Experiment: Multiwavelength excitation Raman measurements

Defect identification

Secondary phase identification: phase diagram

Structure-function correlation: Device performance

high crystal quality, stoichiometric samples

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Lattice Dynamics Calculations

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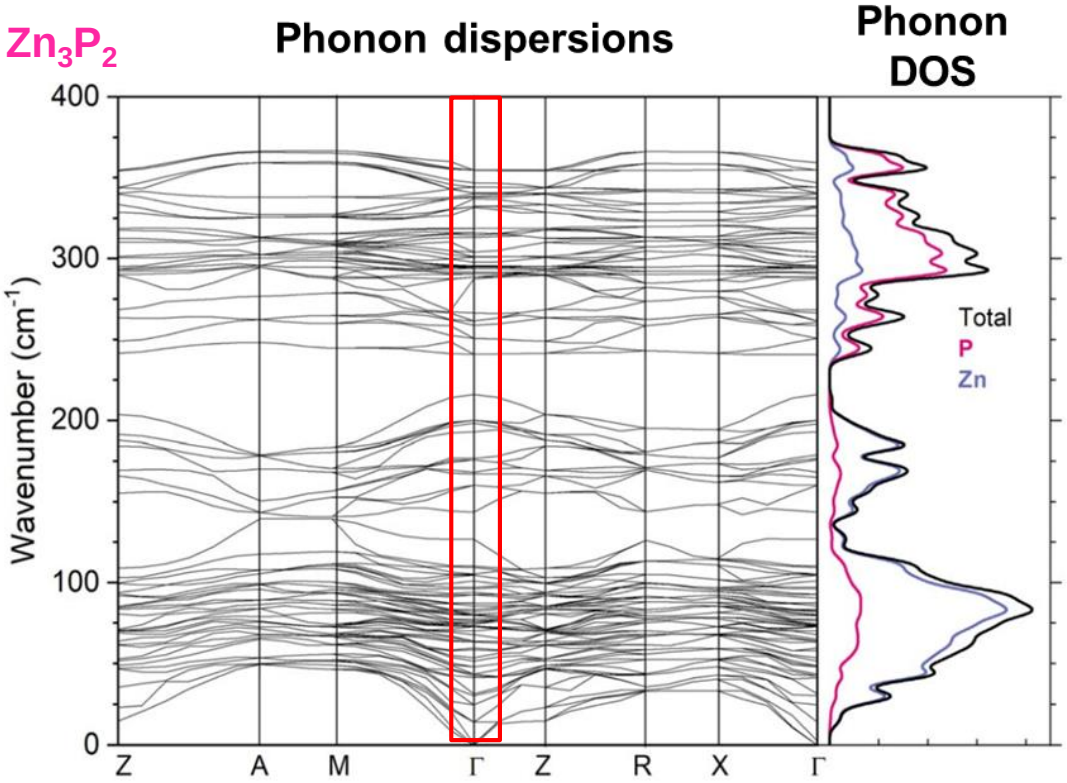
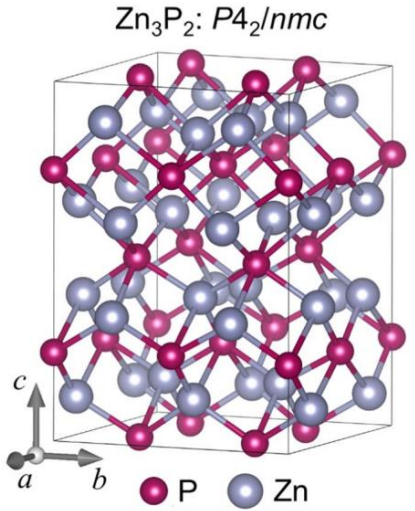
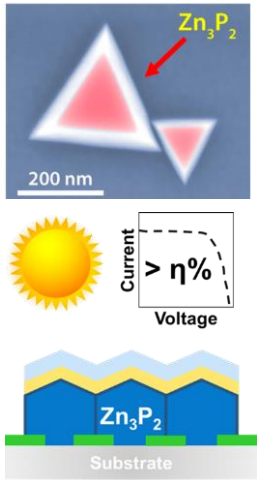
Zn_3P_2







Irreducible representation:

$$\Gamma_{total} = 9A_{1g} + 5A_{2g} + 10B_{1g} + 4B_{2g} + 16E_g + 4A_{1u} + 10A_{2u} + 5B_{1u} + 9B_{2u} + 16E_u,$$

$$\Gamma_{Raman} = 9A_{1g} + 10B_{1g} + 4B_{2g} + 16E_g,$$

$$\Gamma_{IR} = 9A_{2u} + 15E_u,$$

E.S. Stutz…M. Dimitrievska, Nanotechnology 32 085704 (2021)
M. Flor…M. Dimitrievska, Phys. Chem. Chem. Phys. 24 63 (2022)

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Lattice Dynamics Calculations

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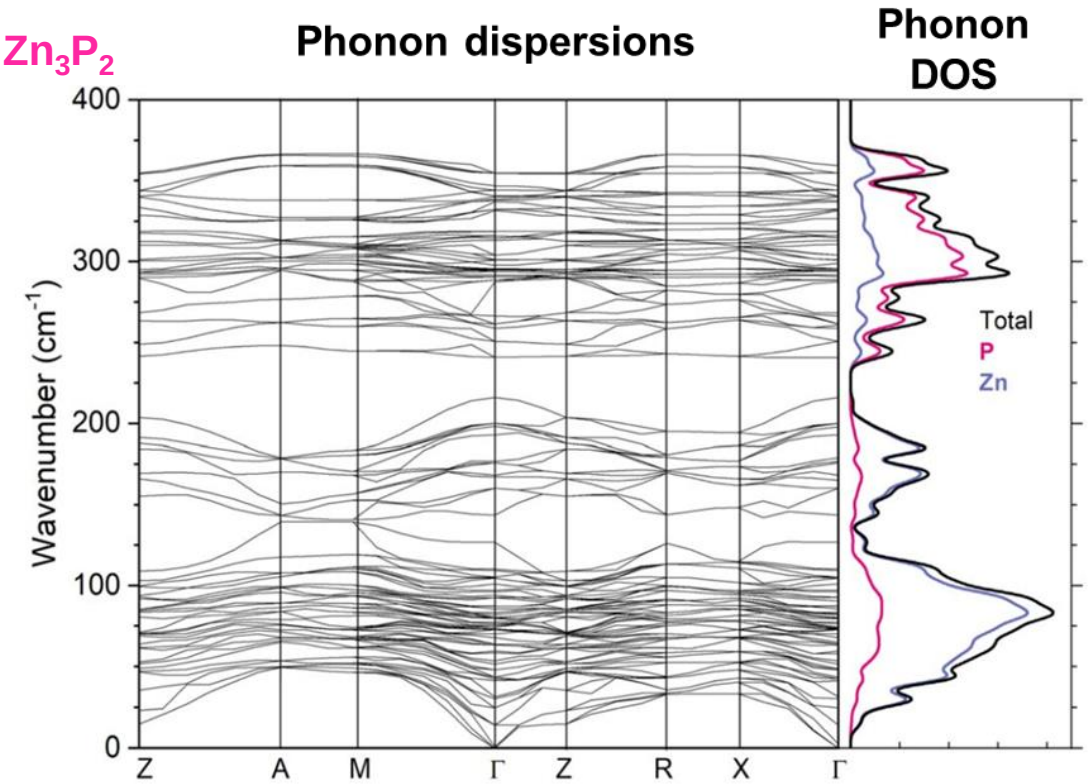
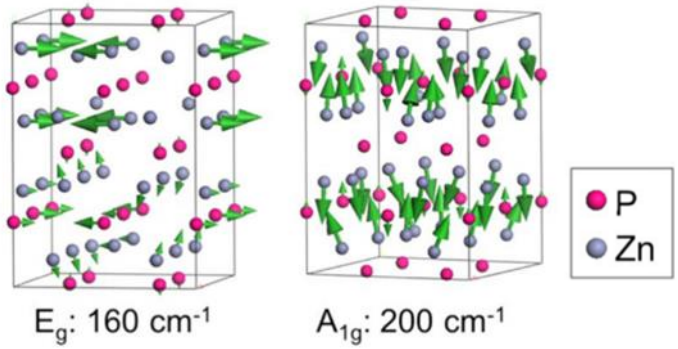
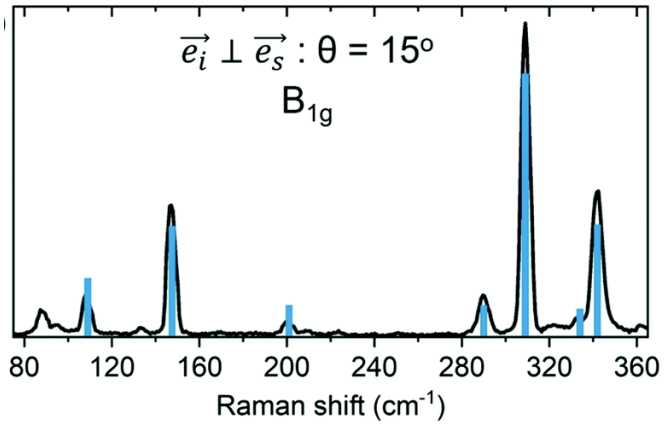
Zn_3P_2



Vibrational patterns



Simulated Raman spectra



E.S. Stutz…M. Dimitrievska, Nanotechnology 32 085704 (2021)
M. Flor…M. Dimitrievska, Phys. Chem. Chem. Phys. 24 63 (2022)

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Materials design roadmap: Raman perspective

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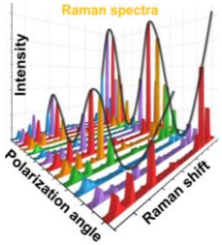
Reference Raman studies

Applied Raman studies

?

Theory: Lattice dynamics calculations



Experiment: Polarization Raman measurements

Experiment: Multiwavelength excitation Raman measurements

Defect identification

Secondary phase identification: phase diagram

Structure-function correlation: Device performance

high crystal quality, stoichiometric samples

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Experiment: synthesis of new materials

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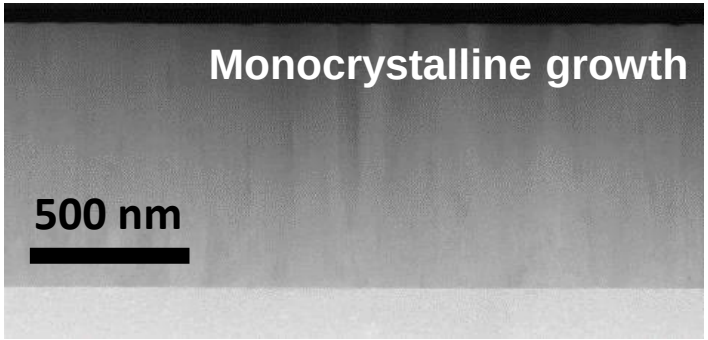
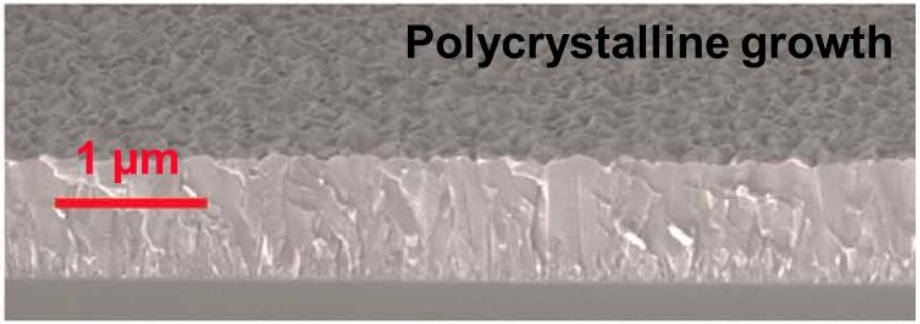
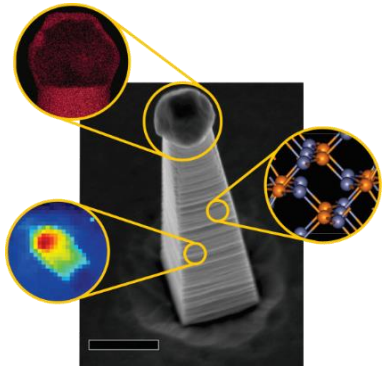
Desired



Usually obtained



Solution:
Nanowires



Advantage:
Single crystal growth

Disadvantage:
Characterization

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M. Dimitrievska et al. Adv. Funct. Mater. 31, 2105426 (2021)

Experiment: Reference Raman spectra

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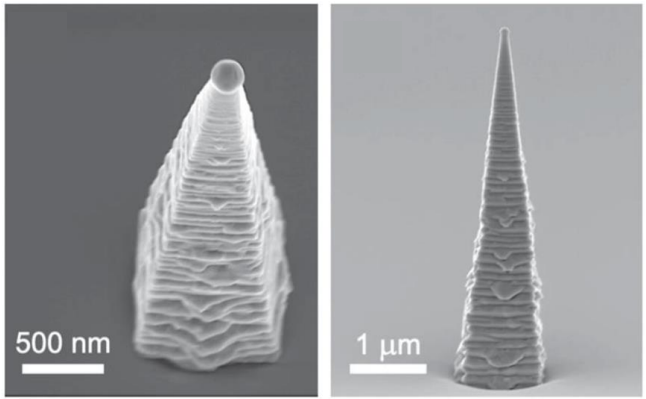
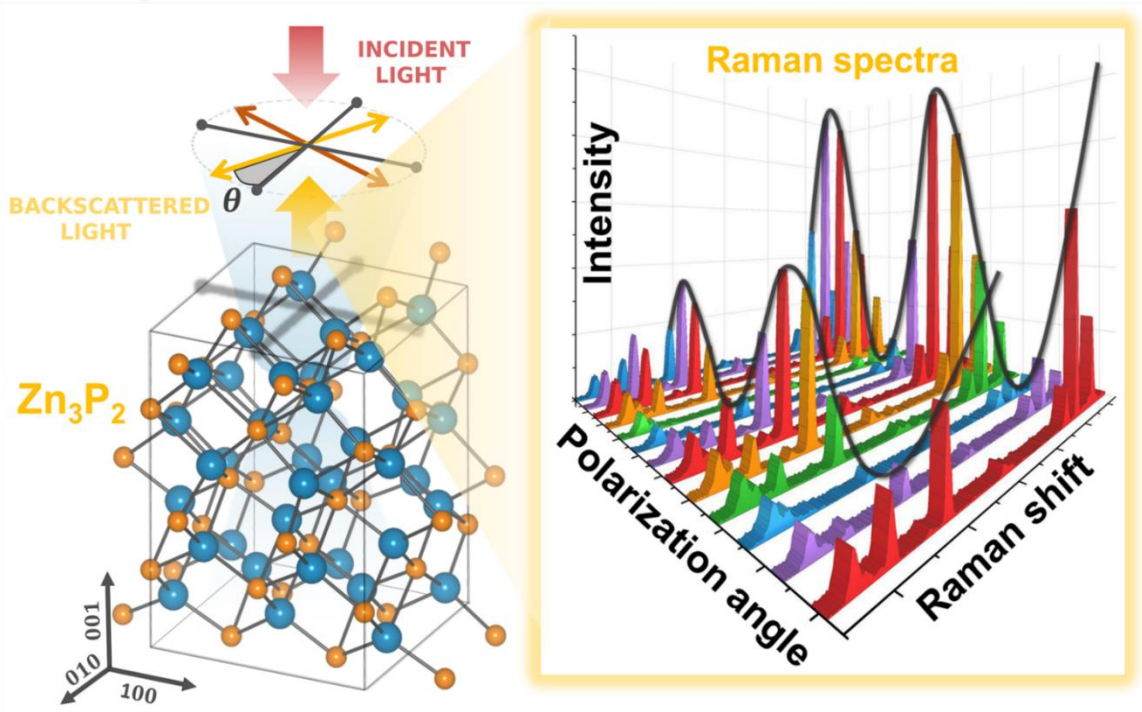
Zn_3P_2 vertical nanowires



Polarization Raman spectroscopy



Raman tensor

$$\Re_{A_{1g}} = \begin{pmatrix} a & 0 & 0 \\ 0 & a & 0 \\ 0 & 0 & b \end{pmatrix}$$

Raman intensity

$$I_S \propto C(\omega_p)\left|\vec{e_i} \cdot \Re \cdot \vec{e_S}\right|^2$$

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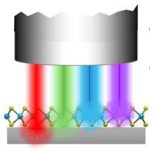
M. Flor…M. Dimitrievska, Phys. Chem. Chem. Phys. 24 63 (2022)



Experiment: Polarization Raman spectroscopy

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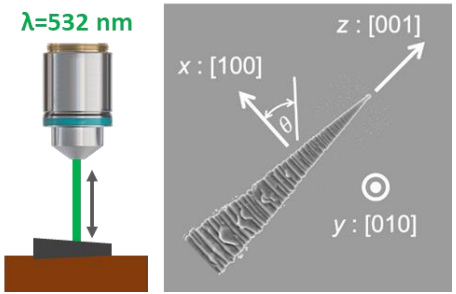
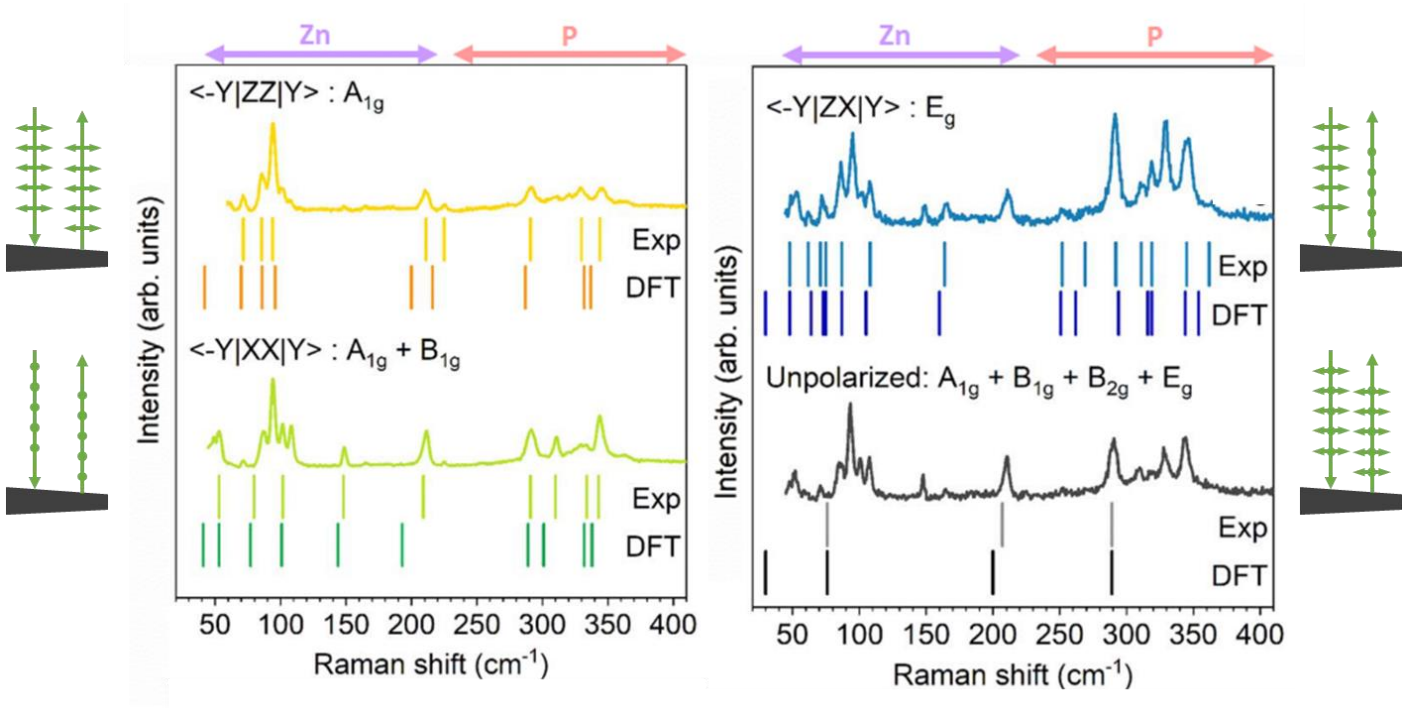
Measurements geometry





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M. Flor…M. Dimitrievska, Phys. Chem. Chem. Phys. 24 63 (2022)

Identification of peak positions: deconvolution of Raman spectra

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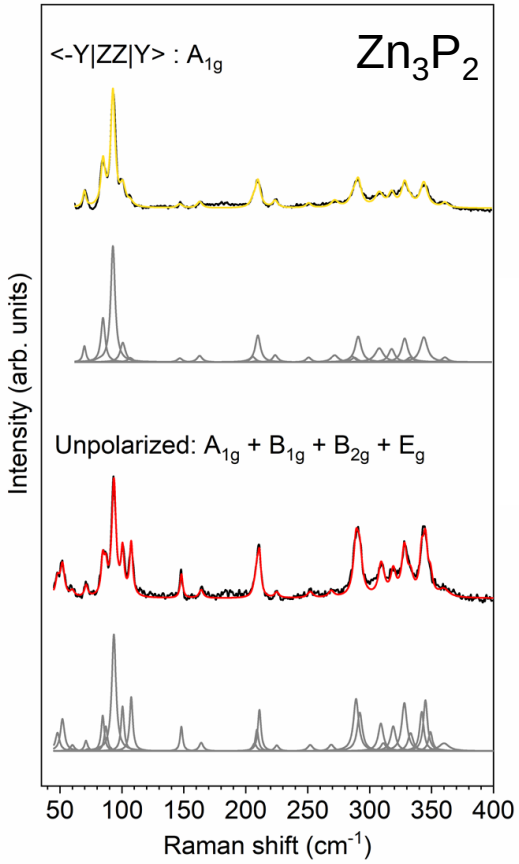
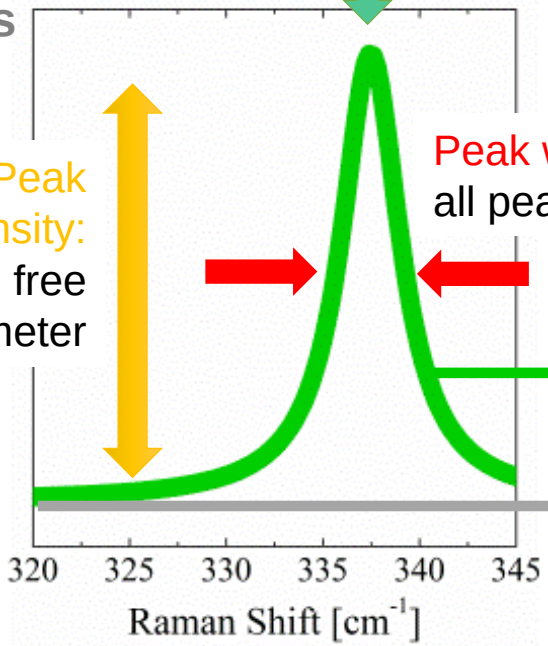


Minimum number of meaningful peaks

Peak positions: constant for different measurement configurations



Peak intensity: free parameter

Peak widths: similar values for all peaks (one phonon modes)

Lorentzian, Gaussian, Voight

Baseline correction

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Materials design roadmap: Raman perspective

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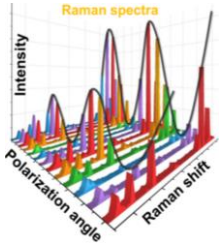
Reference Raman studies

Applied Raman studies

?

Theory: Lattice dynamics calculations



Experiment: Polarization Raman measurements

Experiment: Multiwavelength excitation Raman measurements

Defect identification

Secondary phase identification: phase diagram

Structure-function correlation: Device performance

high crystal quality, stoichiometric samples

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Raman spectroscopy: defect identification

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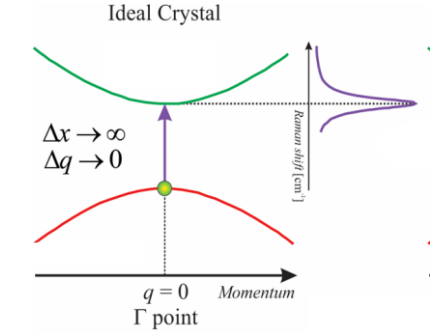

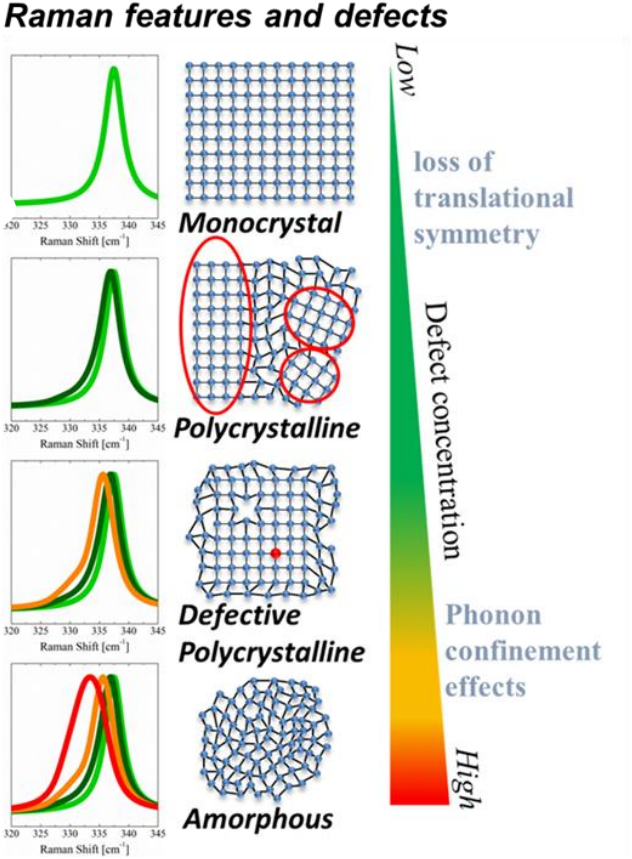

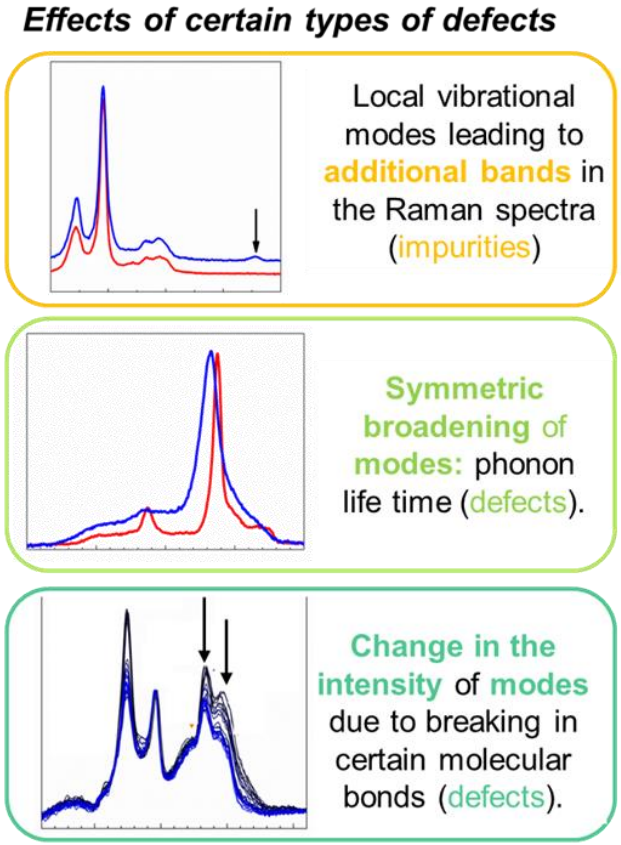

M. Dimitrievska et al., Acta Materialia 70, 272–280 (2014)

M. Dimitrievska et al. Appl. Phys. Lett. 106, 073903 (2015)
M. Dimitrievska et al. J. Mater. Chem. A,7, 13293-13304 (2019)

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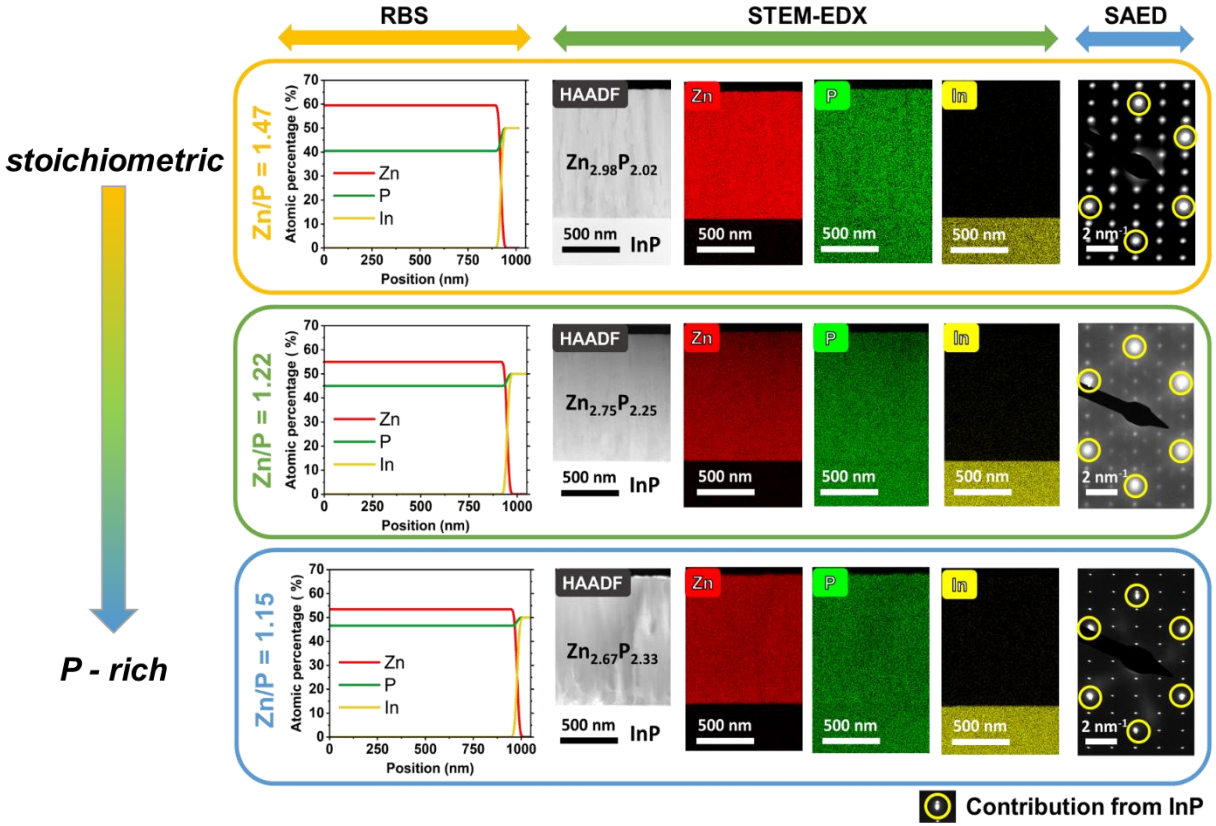
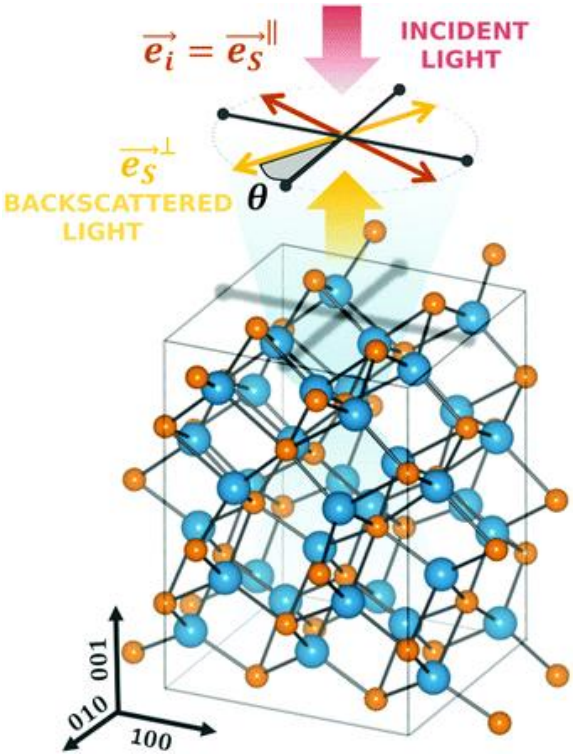
Raman spectroscopy: defect identification

Off-stoichiometric $Zn_{3-x}P_{2+x}$ monocrystalline films





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Raman spectroscopy: defect identification

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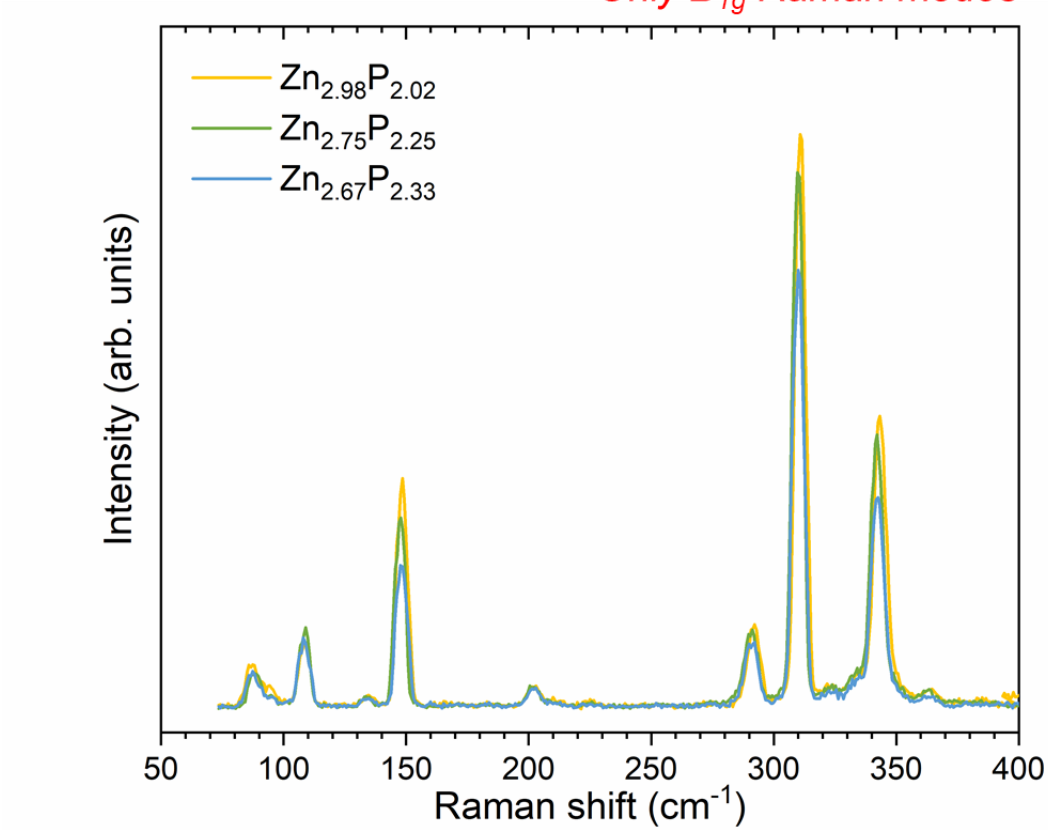
Only B_{1g} Raman modes



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Raman spectroscopy: defect identification

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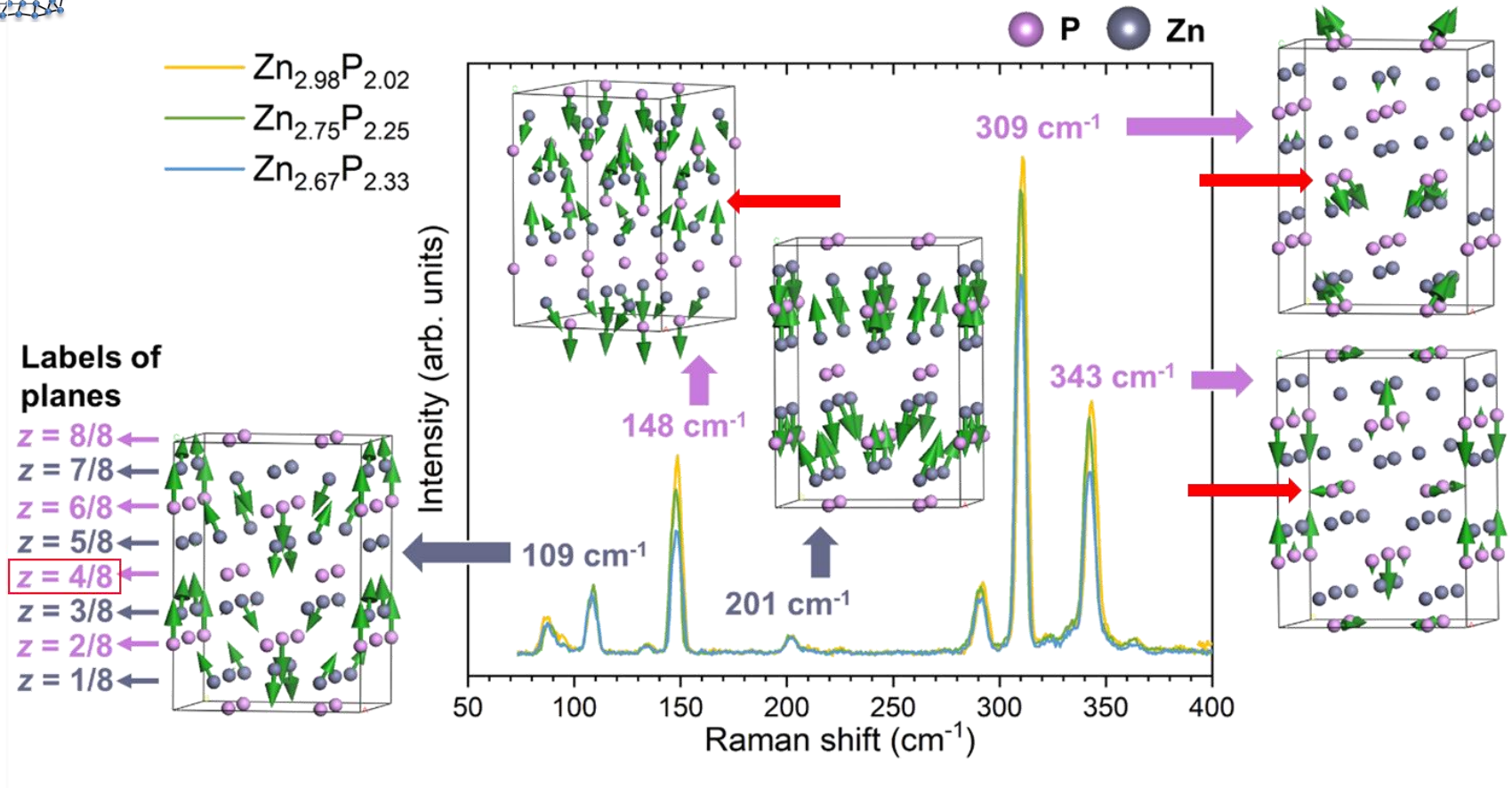

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Raman spectroscopy: defect identification

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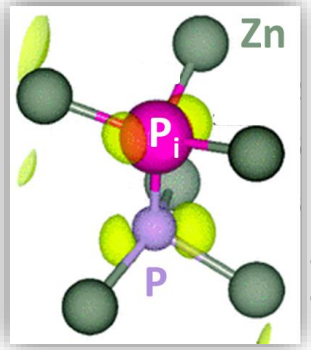
P – interstitials
(DFT defect calculations)



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Raman spectroscopy: defect identification

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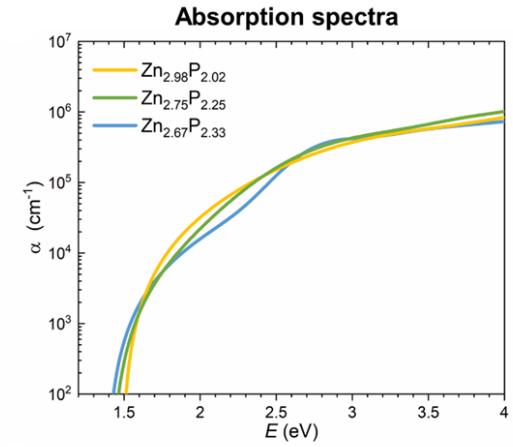
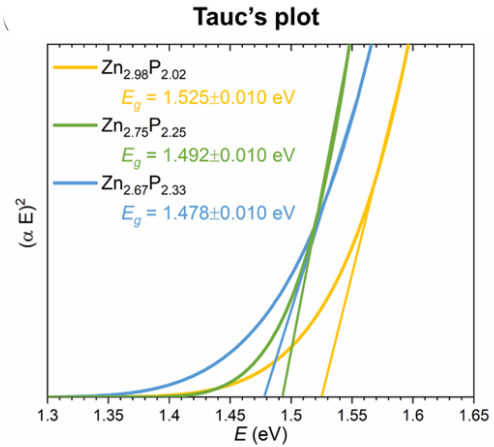
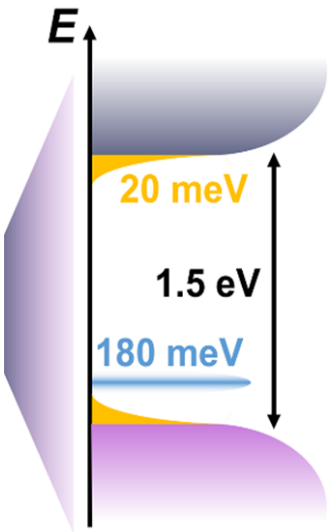
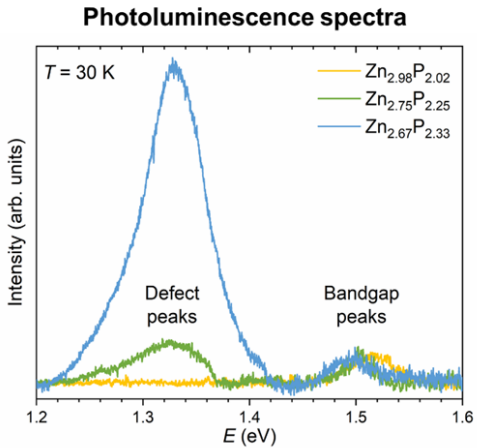
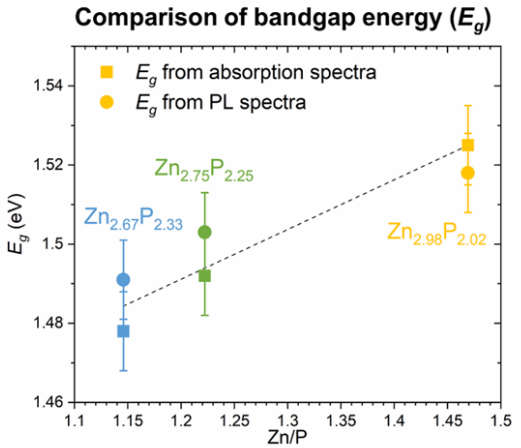
Tunable optoelectronic properties











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Materials design roadmap: Raman perspective

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Materials Science and Technology

Reference Raman studies

Applied Raman studies

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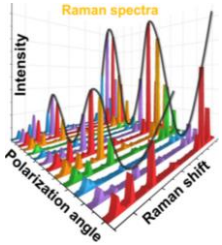
Theory: Lattice dynamics calculations



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Raman spectroscopy: defect identification

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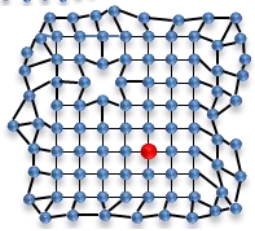
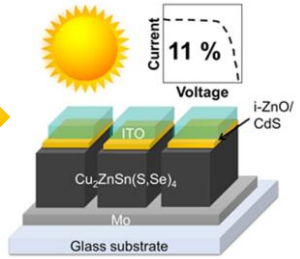
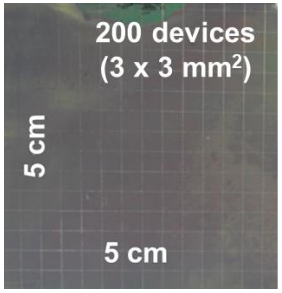
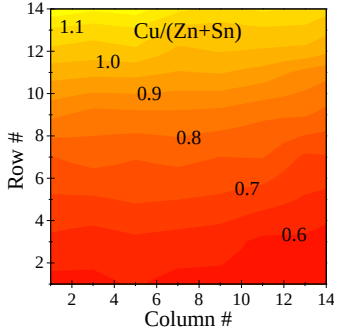


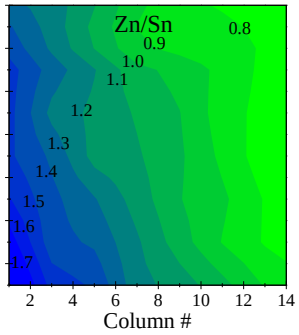
Defects in structure



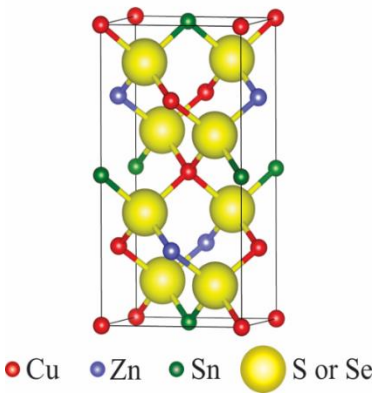
Device performance



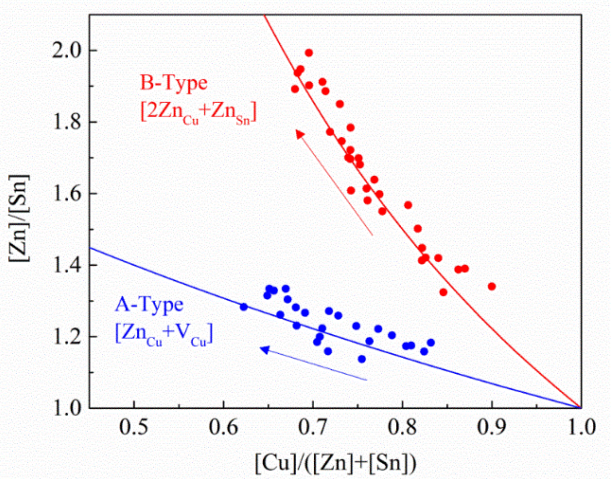




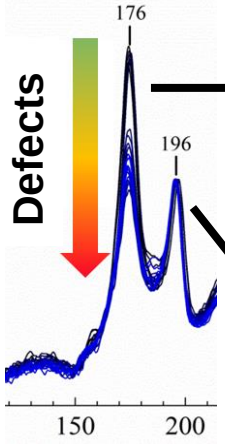
Kesterite: $Cu_2ZnSnSe_4$



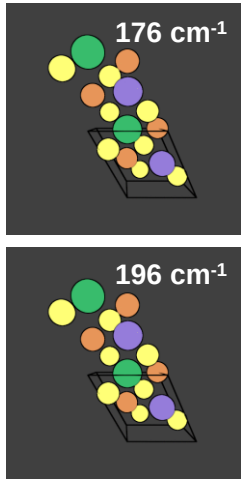
Compositionally induced defects



Experiment



DFT calculations



M. Dimitrievska et al. **J. Mater. Chem. A**,7, 13293-13304 (2019)
M. Dimitrievska et al. **Solar Energy Materials & Solar Cells** 157, 462 (2016)

Raman spectroscopy: defect identification

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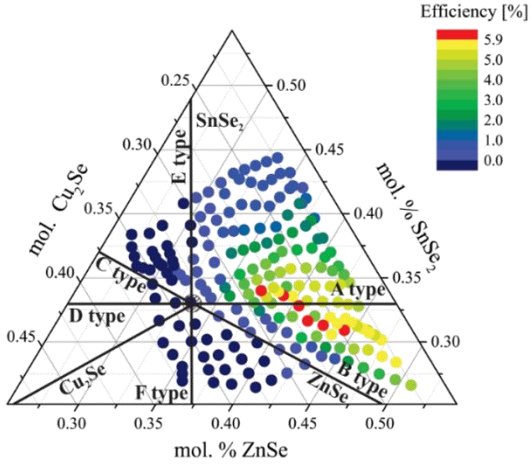
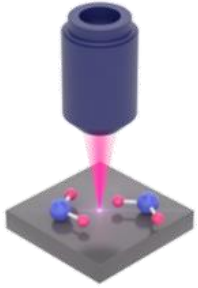
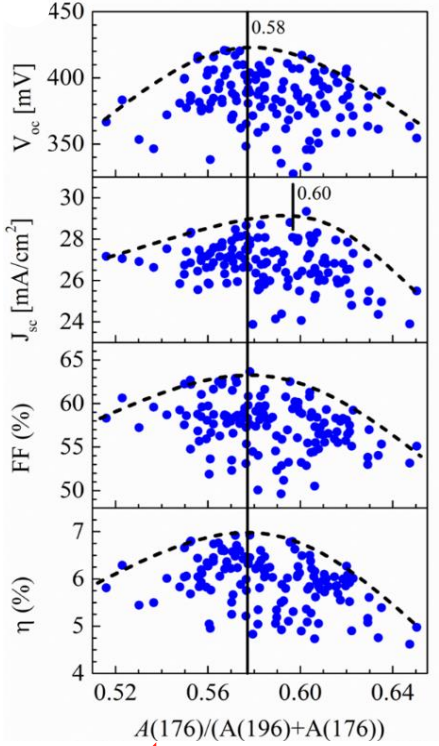
Defect engineering

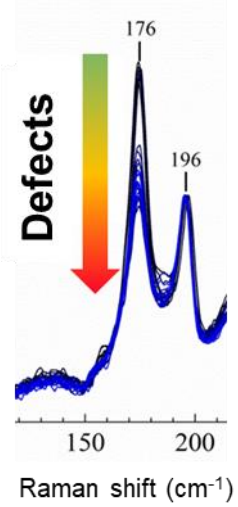


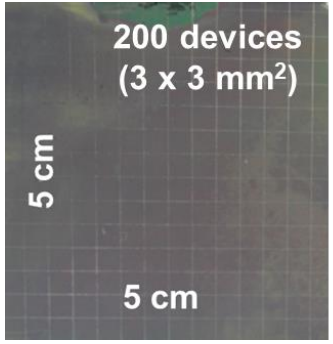
Raman spectroscopy

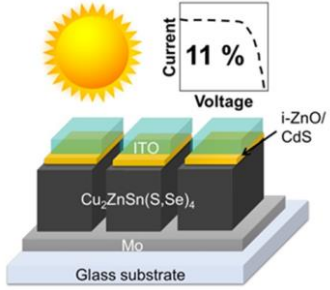


Device performance









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M. Dimitrievska et al. Solar Energy Materials & Solar Cells 157, 462 (2016)

Accelerated materials development

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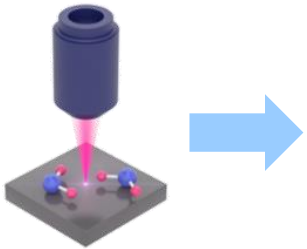
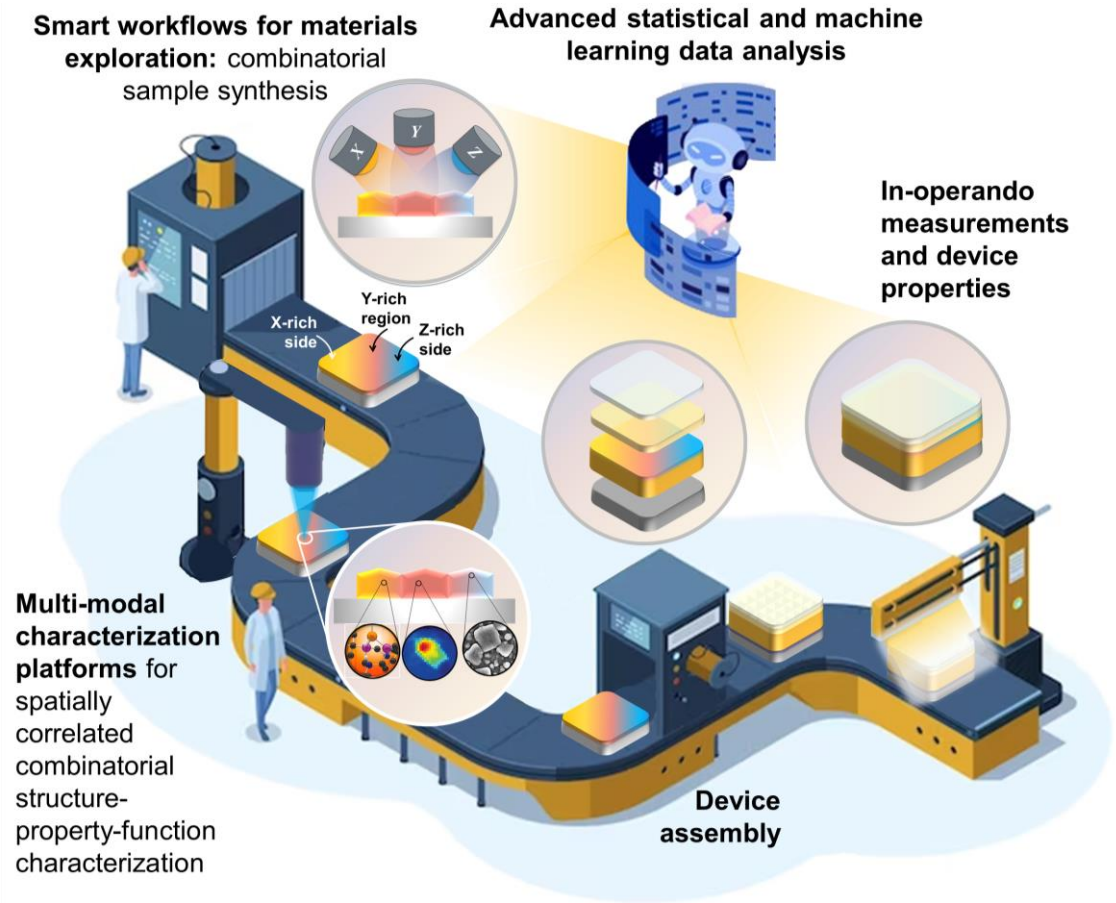


Raman spectroscopy



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M.Dimitrievska,
High-throughput experimentation for accelerated materials development (2023)

Materials design roadmap: Raman perspective

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Reference Raman studies

Applied Raman studies

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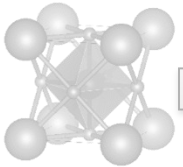
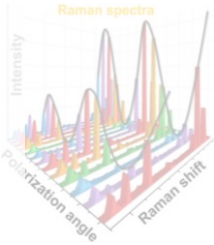
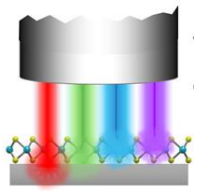


Theory: Lattice dynamics calculations

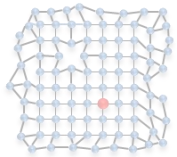


Experiment: Polarization Raman measurements



Experiment: Multiwavelength excitation Raman measurements

high crystal quality, stoichiometric samples



Defect identification

Secondary phase identification: phase diagram

Structure-function correlation: Device performance

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Multiwavelength excitation Raman spectroscopy

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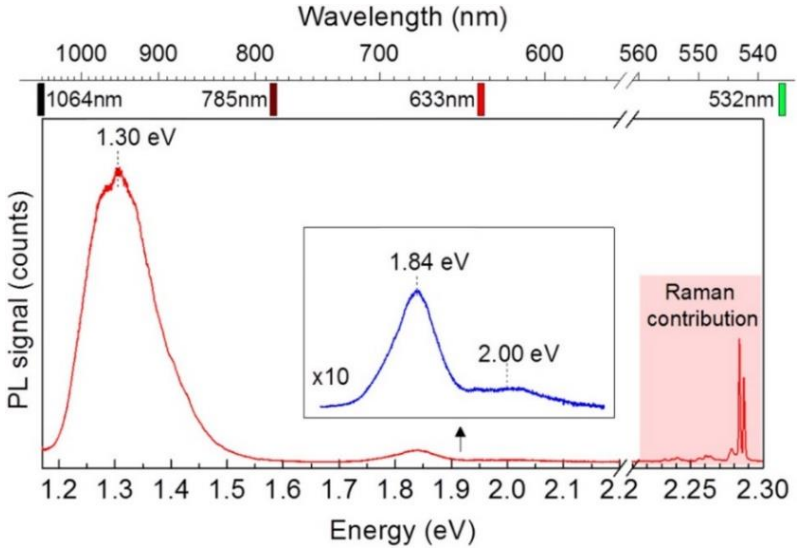
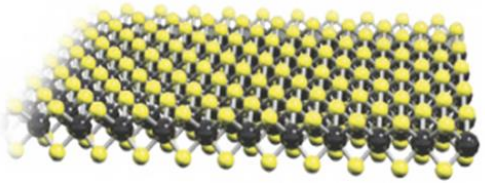
$\lambda_{ext} \approx E_g$ or E_i: **resonance conditions**

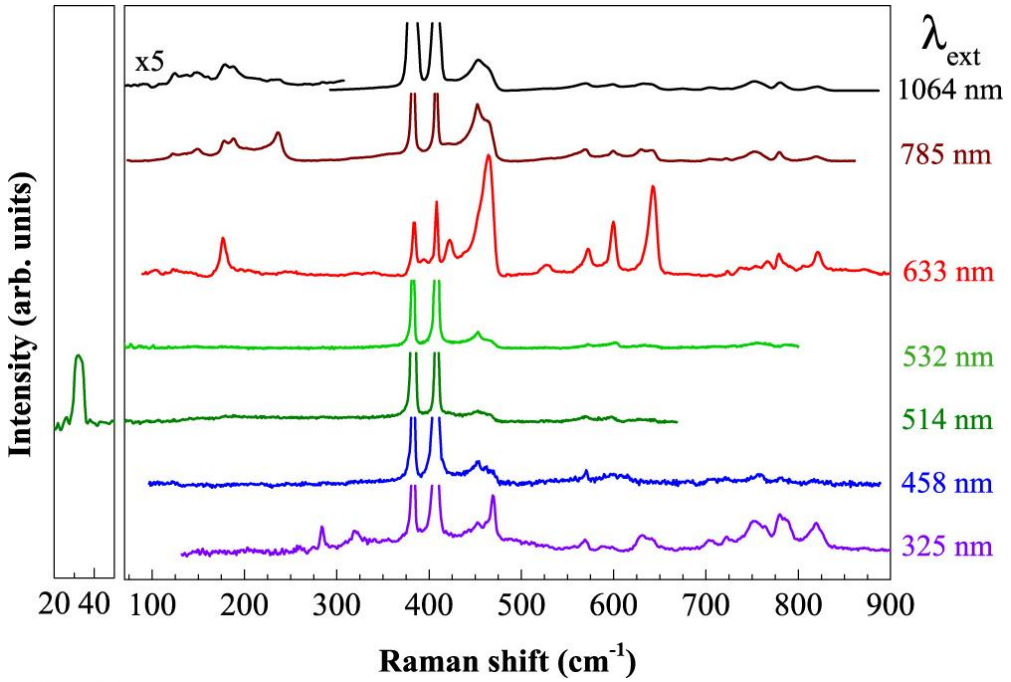
Raman intensity:

$$I \propto \frac{2\pi}{\hbar}\left|\frac{\langle 0|H_{e-r}|n\rangle\langle n|H_{e-Ph}|n'\rangle\langle n'|H_{e-r}|0\rangle}{(\hbar\omega_i-(E_{|n\rangle}-E_{|0\rangle})+i\Gamma)(\hbar\omega_s-(E_{|n'\rangle}-E_{|0\rangle})+i\Gamma)}\right|^2$$



MoS_2 (single crystal)





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M.Placidi, M. Dimitrievska et al. 2D Mater. 2 035006 (2015)

Materials design roadmap: Raman perspective

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Reference Raman studies

Applied Raman studies

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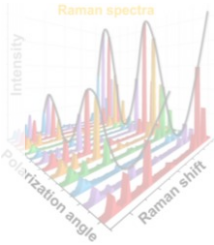
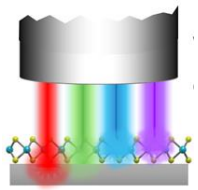
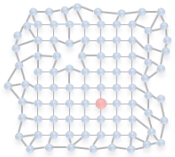
Theory: Lattice dynamics calculations



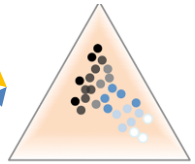
Experiment: Polarization Raman measurements



Experiment: Multiwavelength excitation Raman measurements



Defect identification



Secondary phase identification: phase diagram

Structure-function correlation: Device performance

high crystal quality, stoichiometric samples

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Multiwavelength excitation Raman spectroscopy: impurity identification

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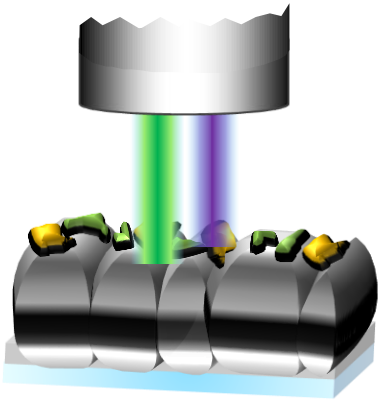
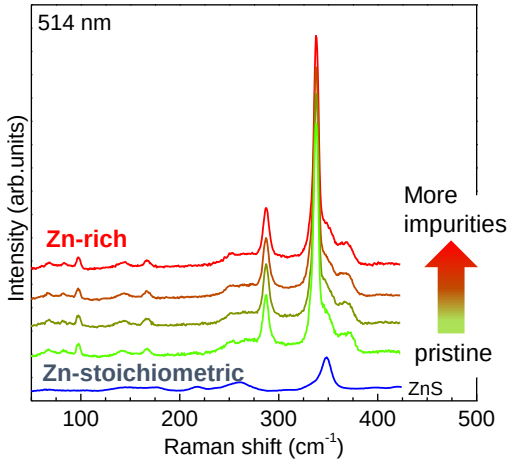
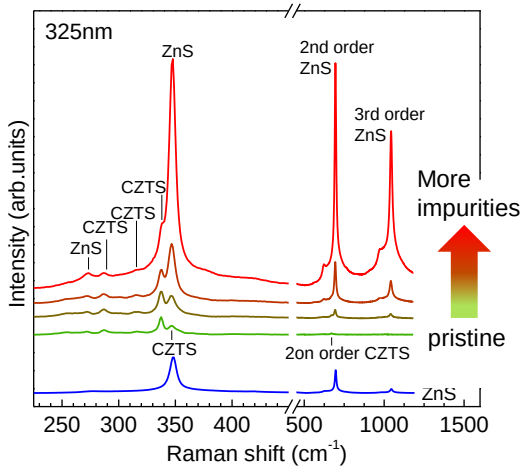
Assessment of ZnS in Cu_2ZnSnS_4



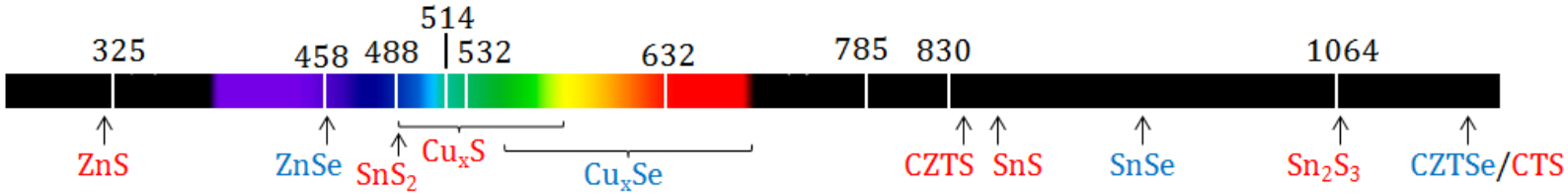
Standard Raman spectroscopy



Resonance Raman spectroscopy



Multiwavelength excitation Raman spectroscopy



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Multiwavelength excitation Raman spectroscopy:

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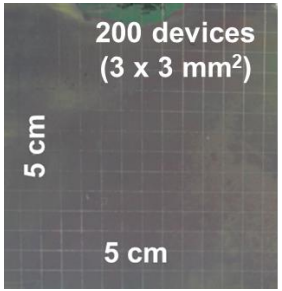
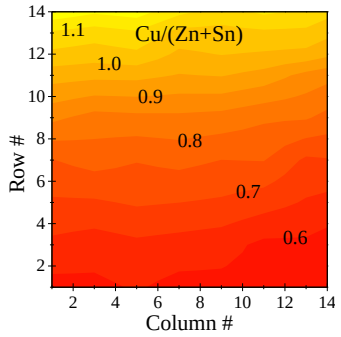
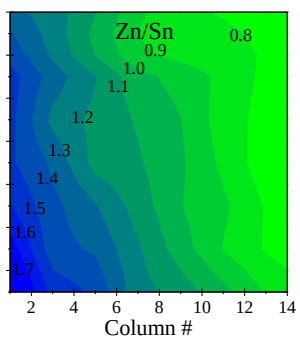
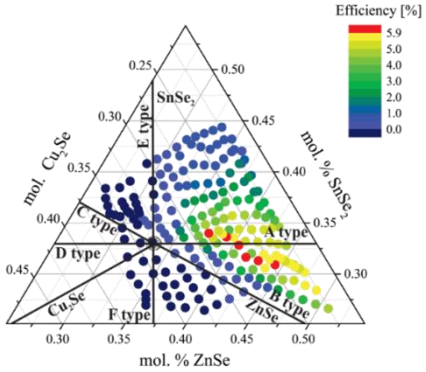
Effect of impurities on the performance of solar cells

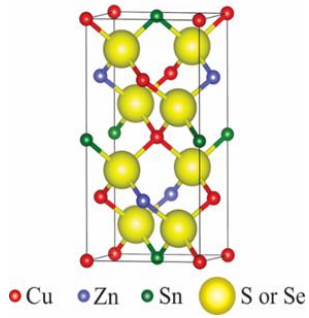








Kesterite: $Cu_2ZnSnSe_4$



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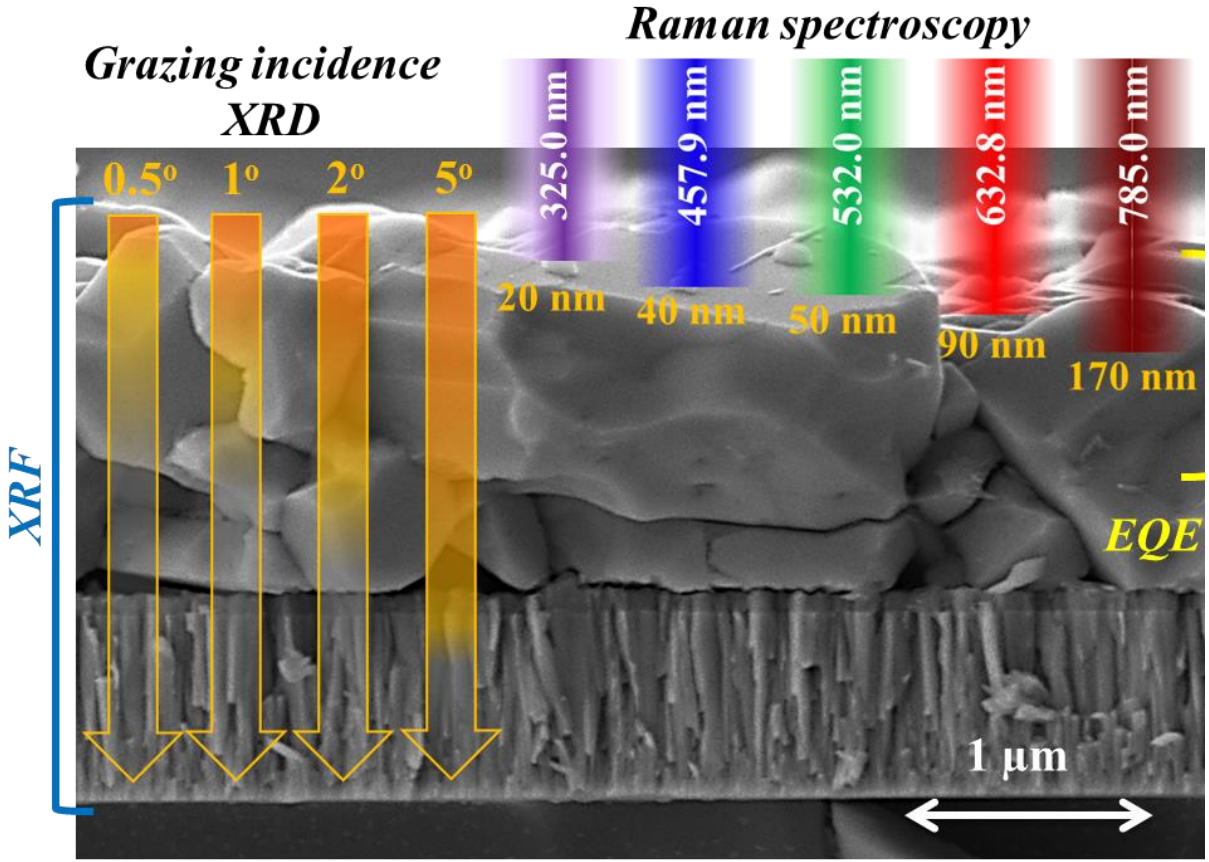
Multiwavelength excitation Raman spectroscopy:



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Multiwavelength excitation Raman spectroscopy:

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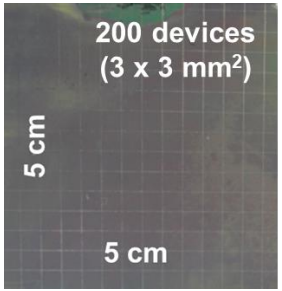
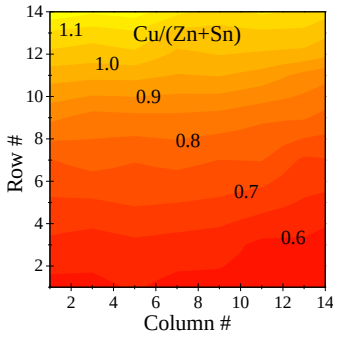
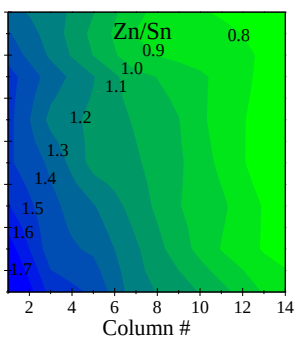
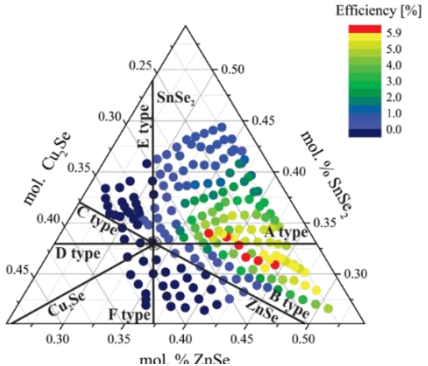
Effect of impurities on the performance of solar cells









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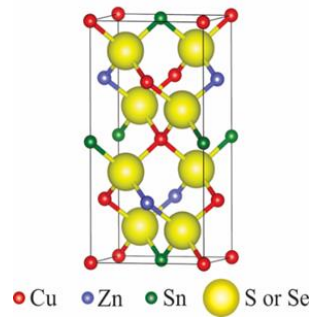
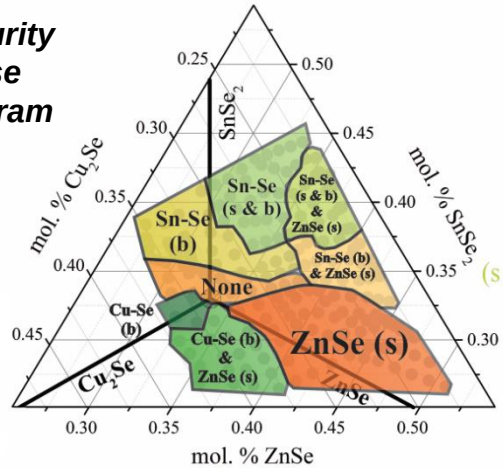
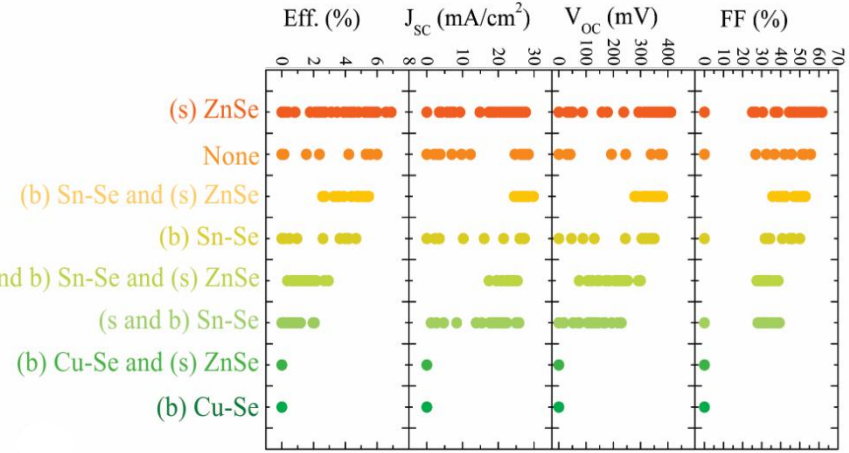


Impurity phase diagram





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Materials design roadmap: Raman perspective

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Reference Raman studies

Applied Raman studies

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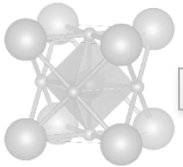
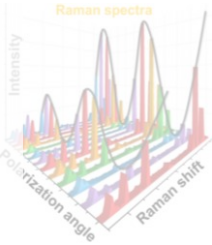
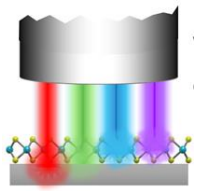


Theory: Lattice dynamics calculations

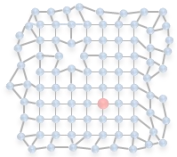


Experiment: Polarization Raman measurements



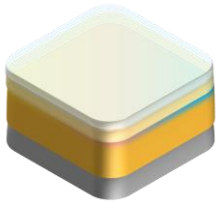
Experiment: Multiwavelength excitation Raman measurements

high crystal quality, stoichiometric samples



Defect identification

Secondary phase identification: phase diagram



Structure-function correlation: Device performance

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Materials design roadmap: Raman perspective

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Reference Raman studies

Applied Raman studies

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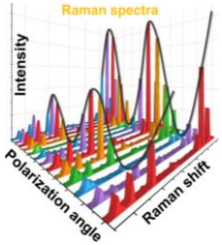
Theory: Lattice dynamics calculations



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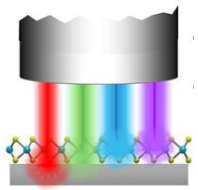
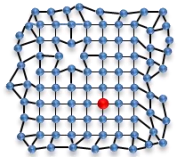
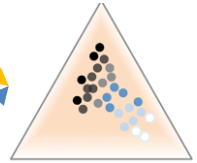


Experiment: Multiwavelength excitation Raman measurements

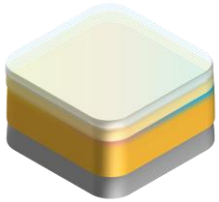
high crystal quality, stoichiometric samples



Defect identification



Secondary phase identification: phase diagram



Structure-function correlation: Device performance

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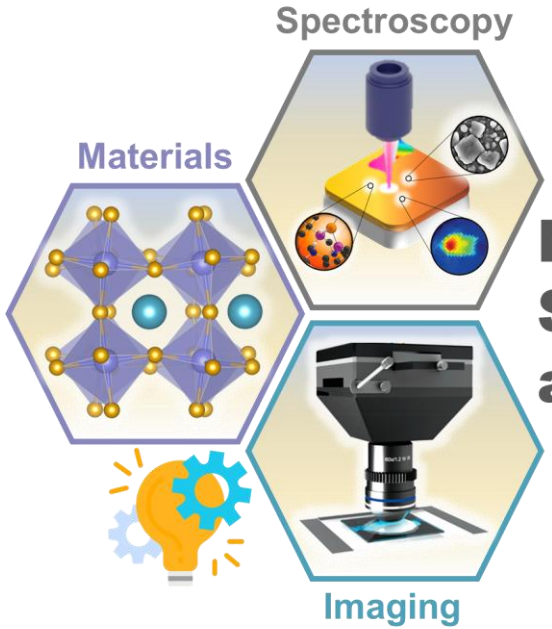
Thank you for your attention!



Nanomaterials Spectroscopy and Imaging

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