Leveraging Gold Plasmonics to Detect Magnetic States in 2D Materials via Raman Spectroscopy

HEMI AEOP Internship Final Presentation

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Outline

- **Background**
  - Raman Spectroscopy & Surface-Enhanced Raman Spectroscopy
  - 2D Materials
- **Improvement of MoS_2 with Gold Nanoparticles (AuNPs) shown in Simulations**
  - Simulation Information
  - Absorption, Scattering, & Electric Field
- **Is it better to have the 2D material above or below the AuNPs?**
  - Simulation Information
  - Absorption, Scattering, & Electric Field
- **Experimentation**
  - Synthesizing AuNPs
  - Synthesized AuNPs results
- **Summary and Future Work**

Background

Raman Spectroscopy

Non-destructive chemical analysis technique that provides information on molecular structure and composition

How it works

- A laser shines on the sample
- Most photons scatter without an energy change → Rayleigh scattering
- Small fraction of photons lose or gain energy due to molecular vibrations → Raman scattering
- The energies of the vibrations are specific to the material's composition and structure

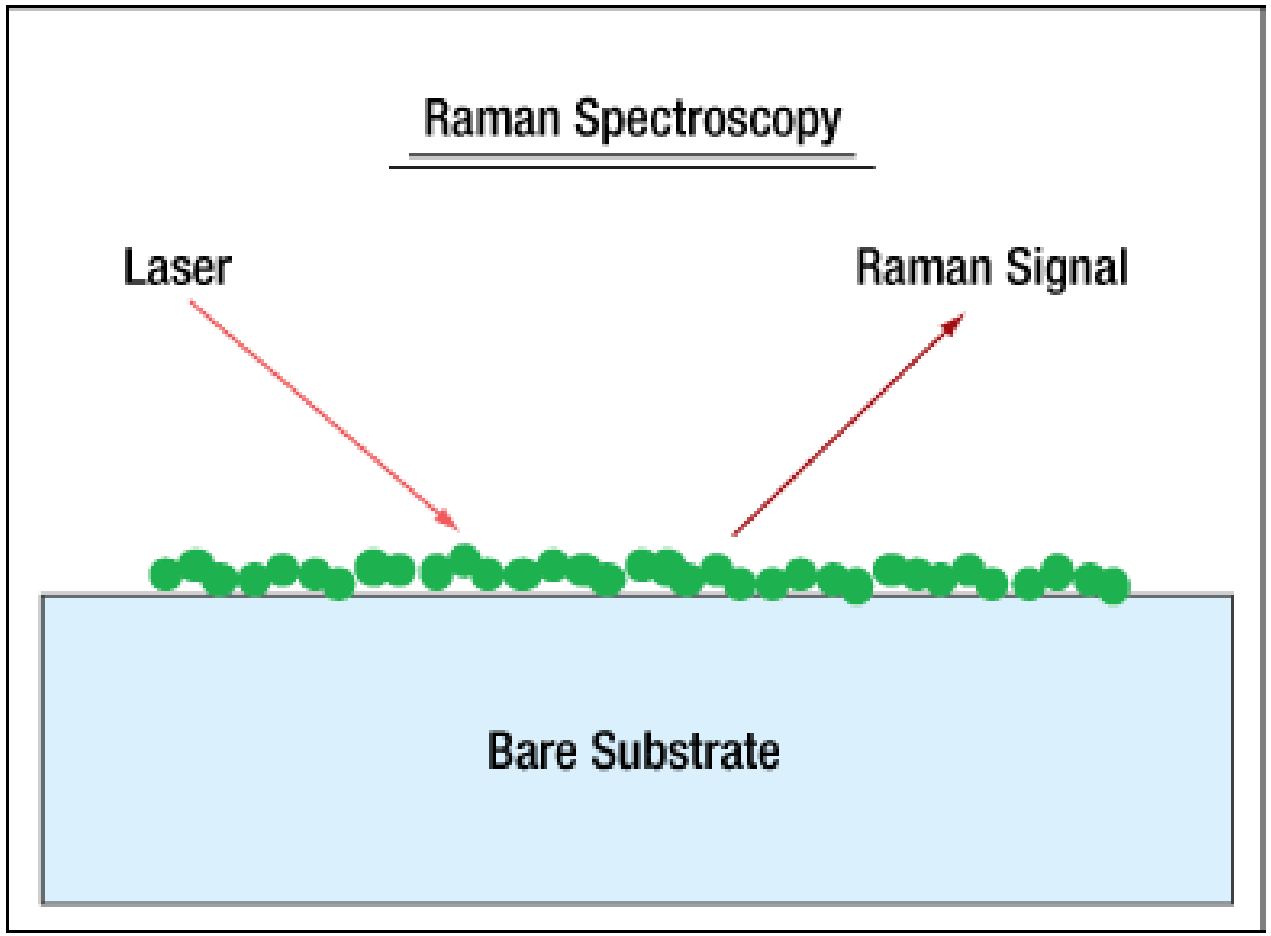

Diagram of Raman Spectroscopy Spectroscopy from Thor Labs [1]

References:
[1] "Surface-Enhanced raman spectroscopy (SERS) substrates." https://www.thorlabs.com/newgrouppage9.cfm?objectgroup_id=16610

Surface-Enhanced Raman Spectroscopy (SERS)

Enhances the Raman scattering signals of molecules close to metallic surfaces

How it works

- Samples are placed on nanoscale metallic surfaces
- Surface plasmons: free electrons on the metal surface oscillate collectively
- When incident light matches plasmon frequency → localized surface plasmon resonance (LSPR) occurs
- LSPR creates intense "hot spots" with very high local electric fields
- These fields amplify the Raman scattering from nearby molecules (the sample)

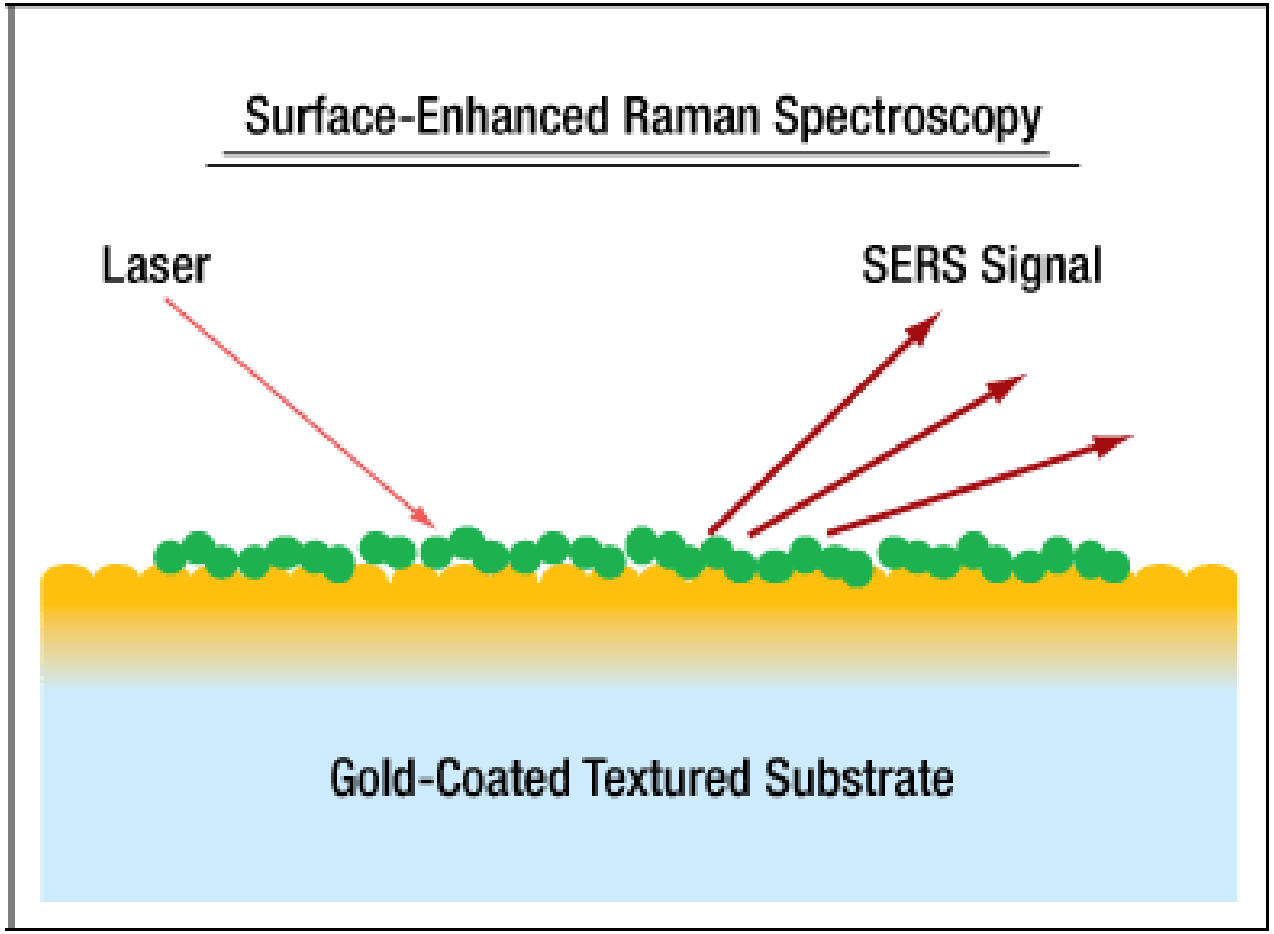

Diagram of Surface-Enhanced Raman Spectroscopy from Thor Labs [2]

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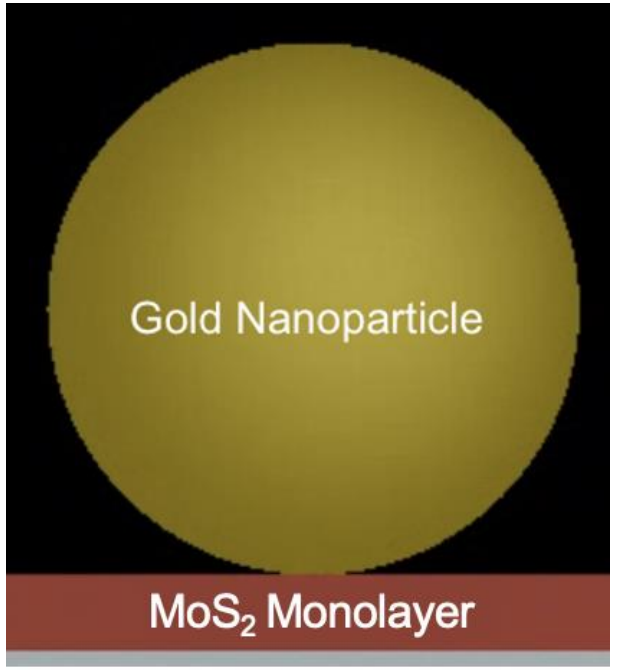
[2] "Surface-Enhanced raman spectroscopy (SERS) substrates." https://www.thorlabs.com/newgrouppage9.cfm?objectgroup_id=16610

2D materials

Van der Waals materials that can be thinned down to a single layer

Why use SERS to analyze them?

- Large surface area for molecule adsorption
- Good optical and electronic properties
- Can enhance the Raman signal by itself (chemical enhancements)



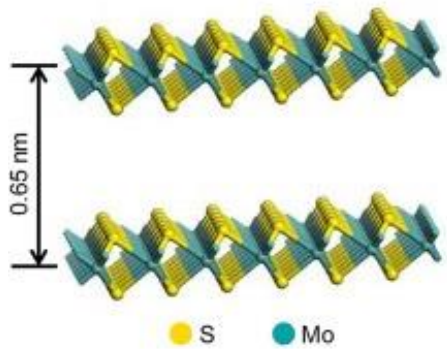


Diagram of MoS_2 [3]

References:
[3] X. Li and H. Zhu, "Two-dimensional MoS2: Properties, preparation, and applications," Journal of Materiomics, vol. 1, no. 1, pp. 33–44, Mar. 2015, doi: https://doi.org/10.1016/j.jmat.2015.03.003.

The problem and our goal

The problem

- Materials with topological surface behavior can theoretically exhibit many new magneto-electric phenomena
  - Applications in spintronics, nonvolatile memory, imaging, metrology, and other on-chip quantum technologies.
- Detecting and controlling spin topological effects is notoriously difficult due to low signals with magnetic techniques

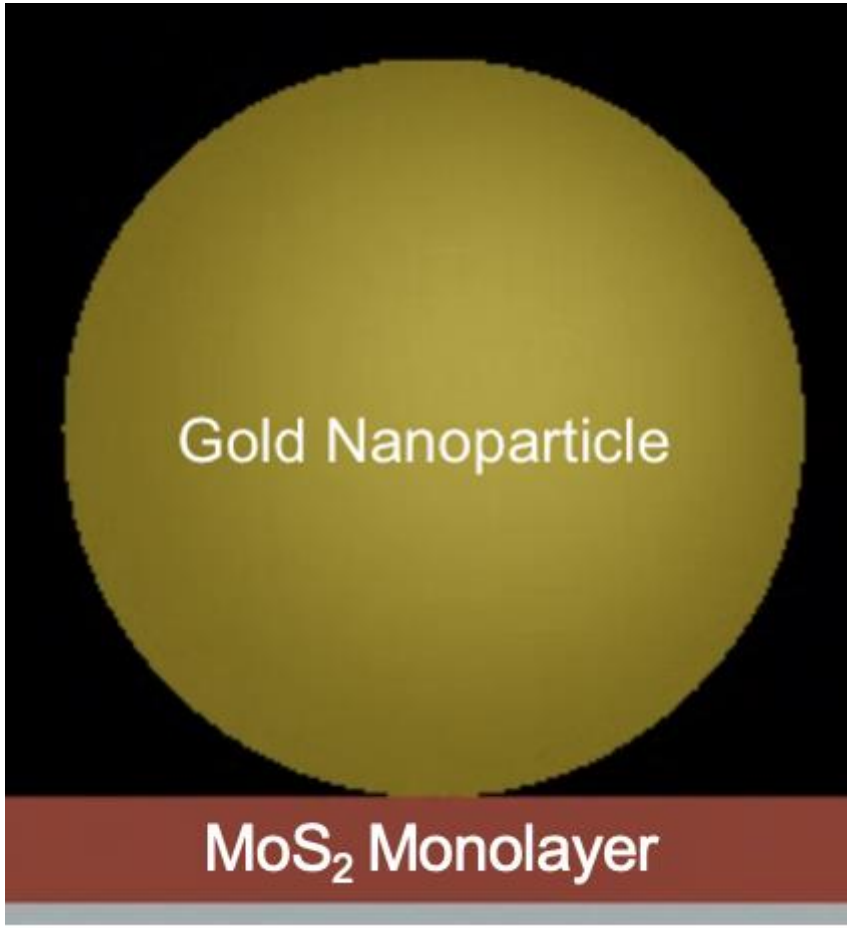
Our goal

- Probe magnetic states of 2D materials using surface-enhanced Raman spectroscopy, completely novel idea
- We hope that the enhancement of Raman spectroscopy will cause visible peaks in the Raman spectra that correspond to magnetic states

Improvement of MoS_2 with Gold Nanoparticles (AuNPs)

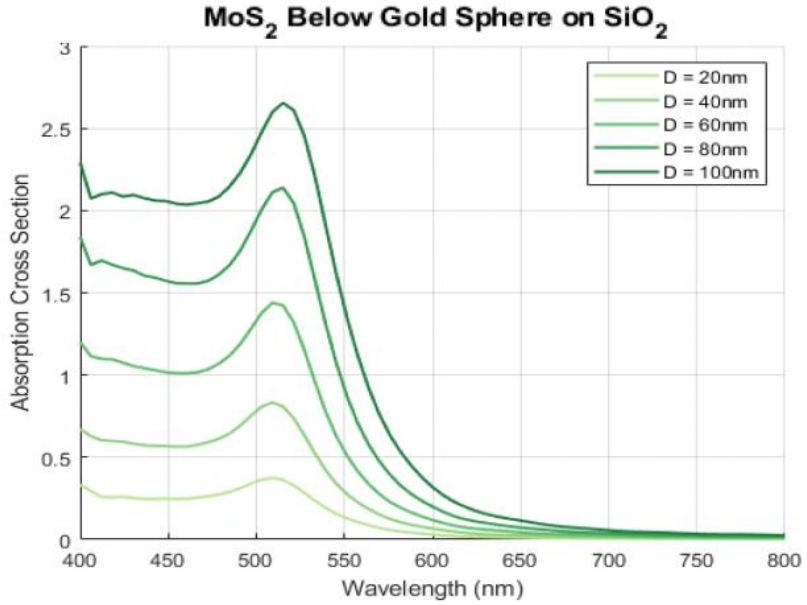
Shown in Lumerical FDTD Simulations

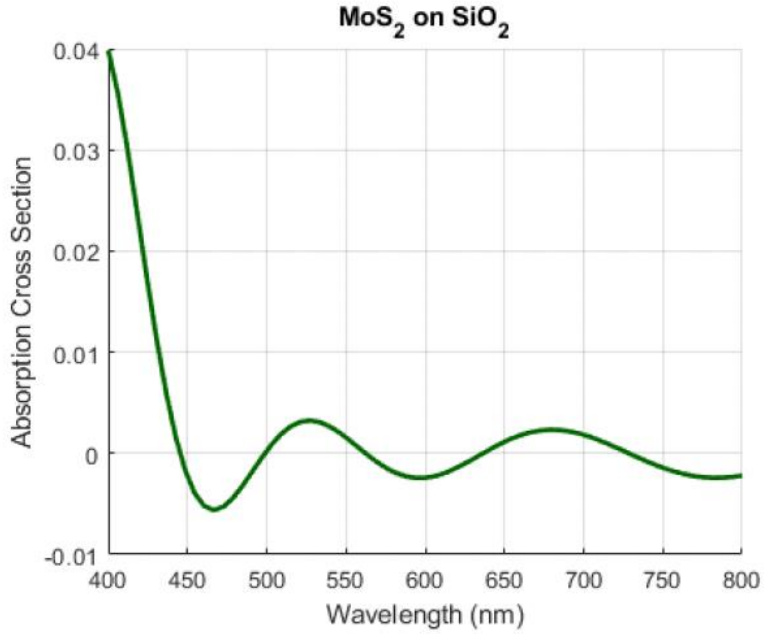
MoS_2 Enhanced with Gold Nanoparticles



2D material below AuNP

Absorption





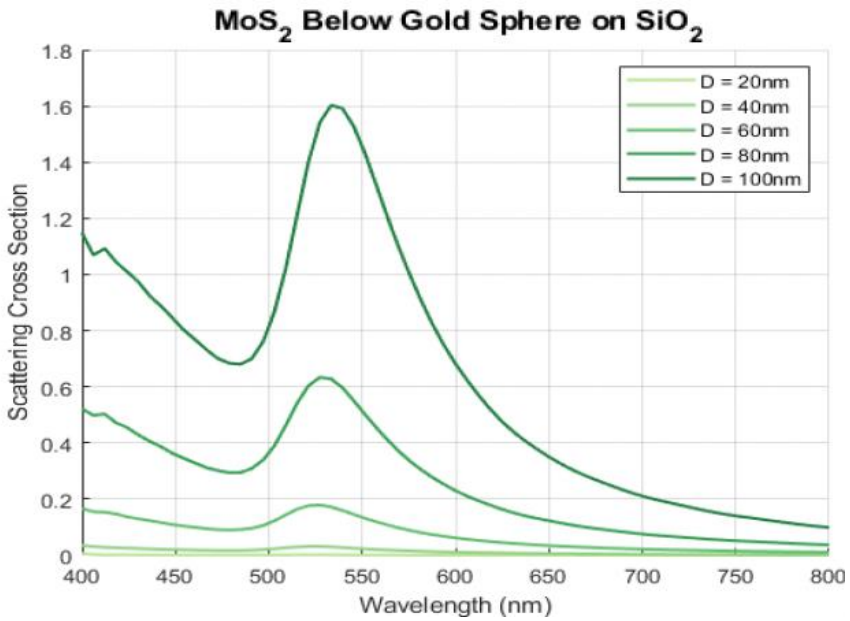
With AuNP's

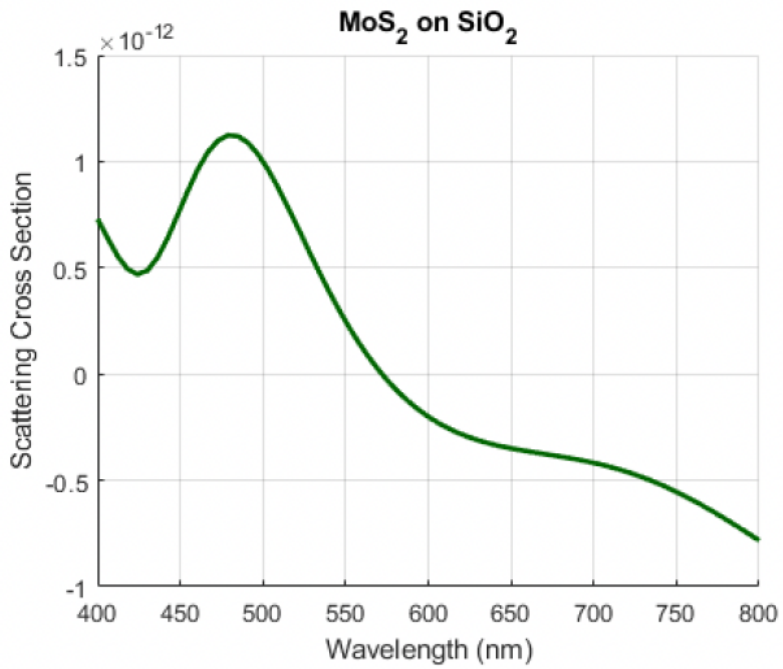
Enhancement in absorption of MoS_2 with gold nanoparticles of varying diameter.

Without AuNP's

Absorption of MoS_2 without gold nanoparticles.

Scattering





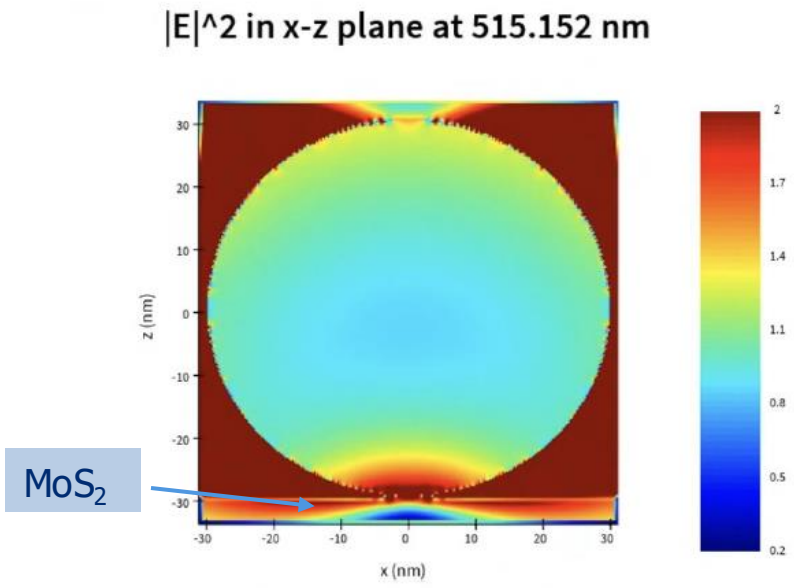
With AuNP's

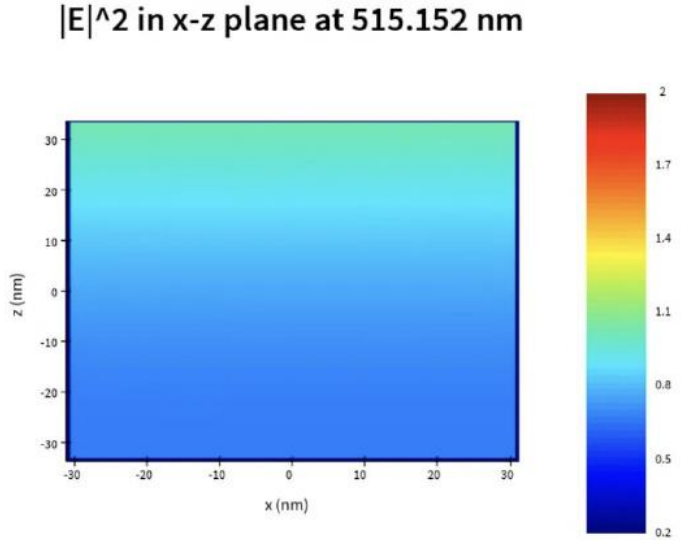
- Enhancement in scattering of MoS2 with gold nanoparticles of varying diameter.

Without AuNP's

- Scattering of MoS2 without gold nanoparticles.

Electric field





With AuNP's

- Electric field intensity in a gold nanoparticle above a thin sheet of MoS_2. Red corresponds to the highest electric field intensity.

Without AuNP's

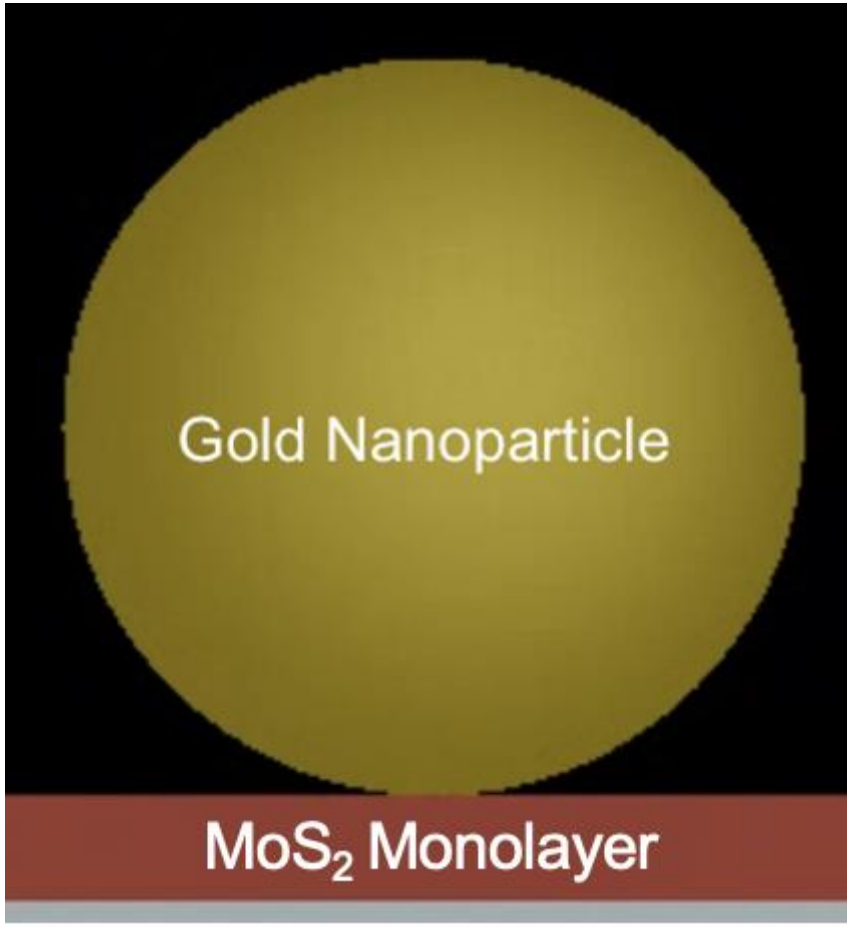
- Electric field intensity in bare MoS_2

Is it better to have the 2D material above or below the AuNPs?

Shown in Lumerical FDTD Simulations

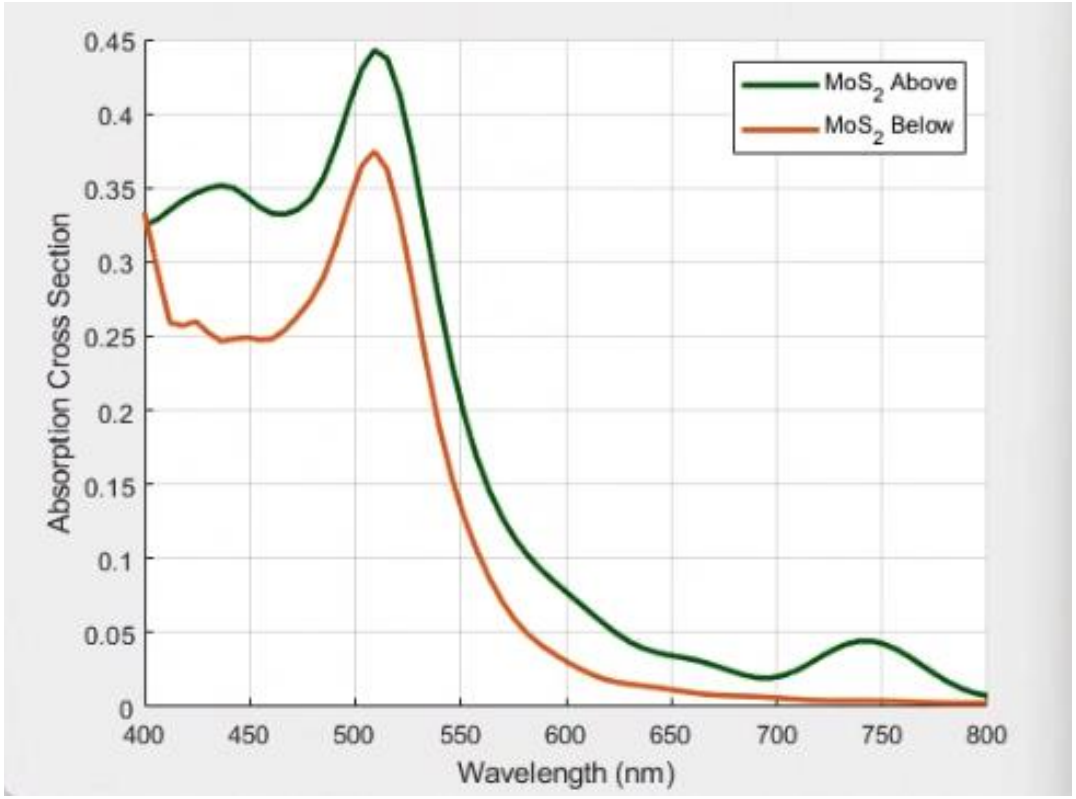
2D material above and below AuNPs

2D material above AuNP

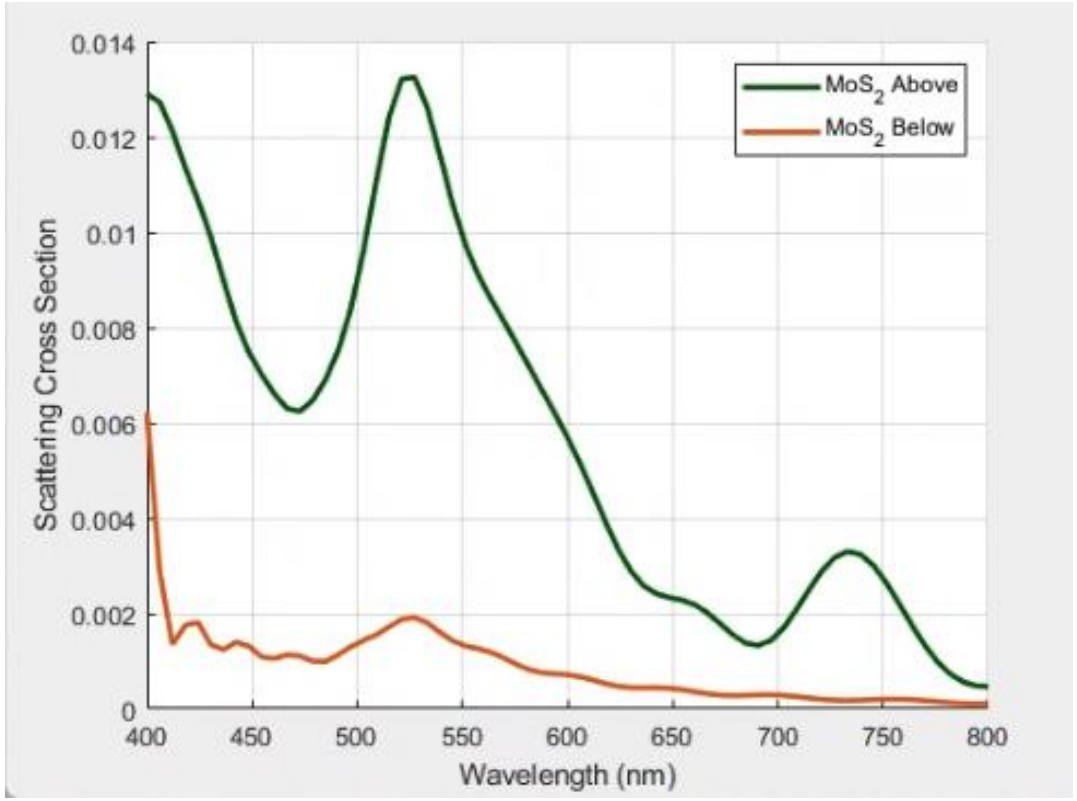


2D material below AuNP

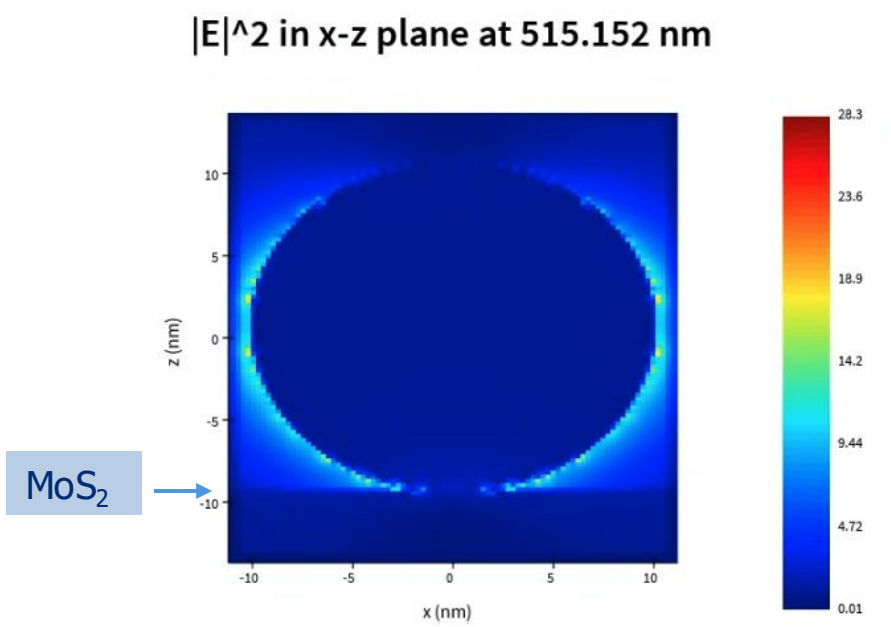
Absorption


0.45
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
Absorption Cross Section
400
450
500
550
600
650
700
750
800
Wavelength (nm)
MoS2 Above
MoS2 Below

Scattering

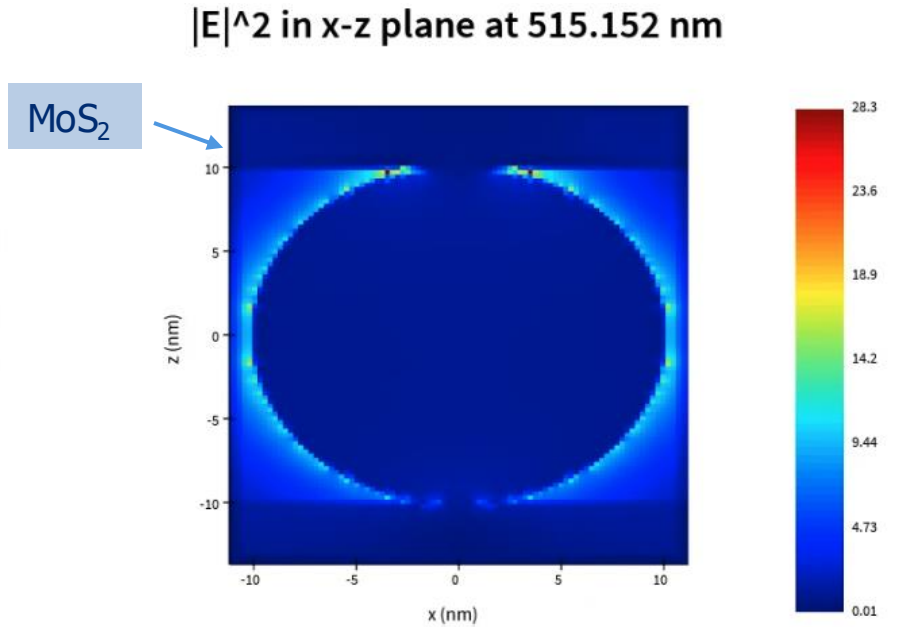

0.014
0.012
0.01
0.008
0.006
0.004
0.002
0
Scattering Cross Section
400
450
500
550
600
650
700
750
800
Wavelength (nm)
MoS2 Above
MoS2 Below

Electric field



2D material below the AuNPs

Maximum Enhancement 17.7655



2D material above the AuNPs

Maximum Enhancement 28.3086

Experimentation

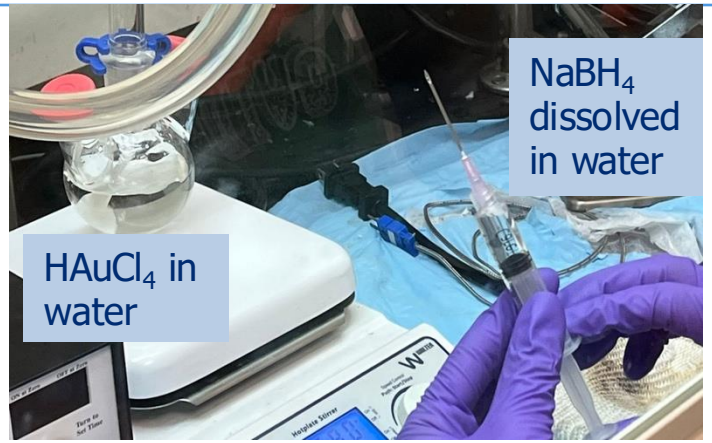
We Synthesized AuNPs

Synthesizing AuNPs

We synthesize gold nanoparticles (AuNPs).

Process:

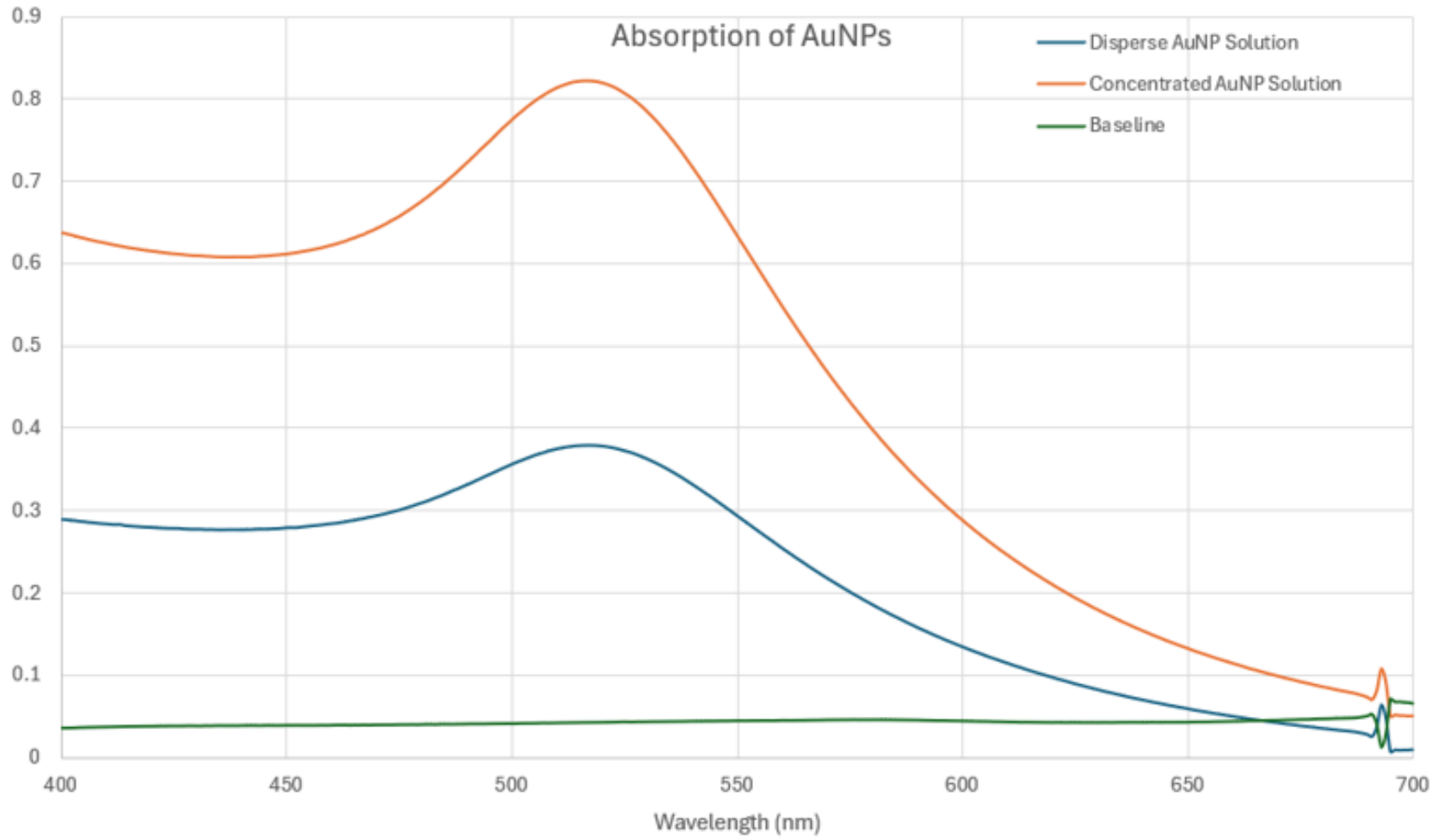
- Adding gold III chloride trihydrate ($HAuCl_4$) to water and mixing under nitrogen
- Stirring in sodium borohydride ($NaBH_4$) dissolved in water, and continued stirring under nitrogen.
- Before adding $NaBH_4$ solution to $HAuCl_4$ solution, both solutions are clear. After adding the $NaBH_4$ solution to the $HAuCl_4$ solution, it turned red-pink, a sign of nanoparticle formation.



AuNP's suspended in water

Synthesized AuNPs results

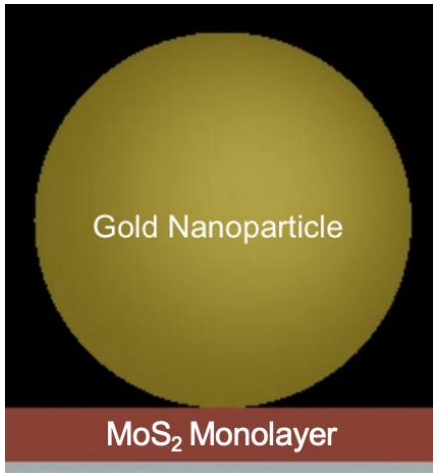
- Peak absorption at wavelengths ~515-525 nm, demonstrating potential for SERS



UV-vis spectra of synthesized AuNPs showing peak absorbance ~525 nm.

Summary and Future Work

- Gold nanoparticles create strong localized electric fields that increase the absorption and scattering of 2D materials due to LSPR enhancement
  - Changing size, spacing, and shape of the nanoparticles can tune the LSPR
- Probe magnetic states of 2D materials using surface-enhanced Raman spectroscopy
  - Continue experimenting to find the best plasmonic structure to use with relevant 2D materials
- Gold plasmonics can also enhance solar cell efficiency
  - Simulations shows that carefully made and deposited gold nanoparticles can enhance light absorption in 2D materials



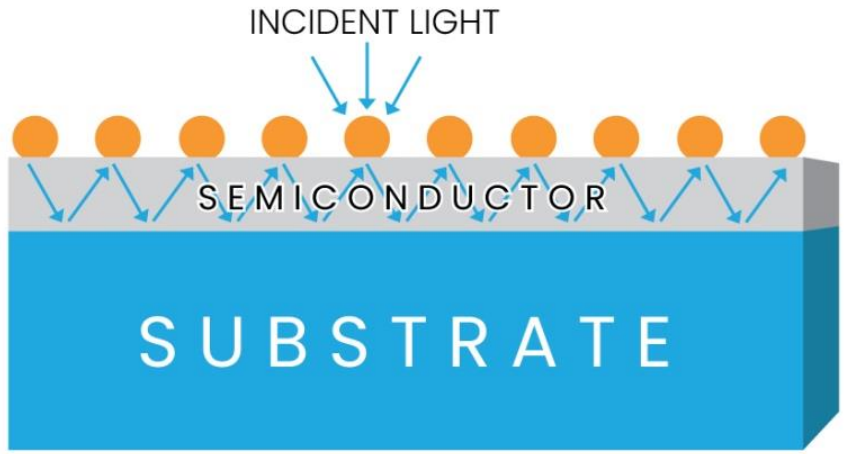


Diagram of a Plasmonic Solar Cell from Sinovoltaics [4].

References
[4] Niclas, "Plasmonic solar cells," *Sinovoltaics (Hong Kong Office)*, Mar. 29, 2023.https://sinovoltaics.com/learning-center/solar-cells/plasmonic-solar-cells/

Thank You!

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