# Interfacial Contact with Noble Metal - Noble metal and Noble Metal – 2D Semiconductor Nanostructures Enhance Optical

Activity

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Modeling and Simulation

# Photonics

### Background/Relevance

- Nanoantenna-enhanced semiconductors exhibit extraordinary optical properties that allow nanoscale energy modulation (i.e. localized surface plasmon resonance (LSPR) and excitons.
- Applications such as optical switching, drug delivery, environmental sensors and photocatalysis can be derived from strong and weak coupling between plasmons and excitons in transition metal dichalcogenide (TMD)-heterostructures.

#### Innovation

• Distinguishing respective contributions of plasmonic heating and hot electron transfer in noble metal - TMD heterostructures via experimentally and computationally.

#### **Key Results**

- Mapped local electric fields and hot electron transfer in 2D materials in order to distinguish relative thermal and hot electron transfer dissipation from LSPR.
- Distinguished respective contributions of electron transfer and plasmonic heating from DDA simulations.



## Approach

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Produce TMD nanoflakes. Scanning transmission electron microscope (STEM) of the TMD-heterostructures. Perform far- and near-field maps of the TMDheterostructures via Discrete Dipole Approximation (DDA). Compare both computational and experimental optical feature enhancements.

Degree: MS, December 2019



Figure 1. G. T. Forcherio, D.K. Roper. Advanced Optical Materials. **2016**, *4*, 1288-1294

#### Conclusions

 These tools allowed comparison between the metal nanoantenna and the DDA simulations to determine relative contributions of plasmonic heating and hot electron transport to increase LSPRenhanced photocatalysis from the TMD-heterostructure.

#### **Future Work**

• Possible x-ray photoelectron spectroscopy (XPS), atomic force microscopy, and Raman spectroscopy to improve understanding of photoinduced doping of TMDs by metal nanoantennae.

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