



APS SATELLITE  
MEETING AT ICTS

# Stacking-Order-Driven Optical Properties and Layer Parity Dependent Phonon Modes in $\text{ReS}_2$

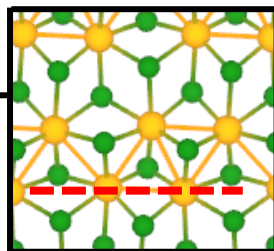
**Nikhilesh Maity**

**March 15, 2022**

**Material Research Centre  
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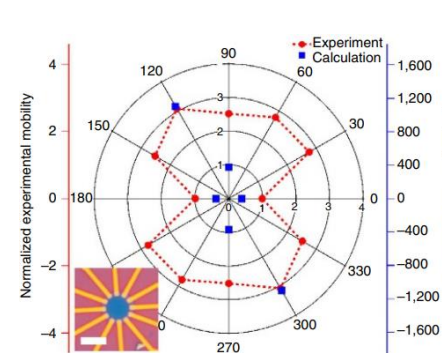
# Uniqueness of ReS<sub>2</sub>

ReS<sub>2</sub>



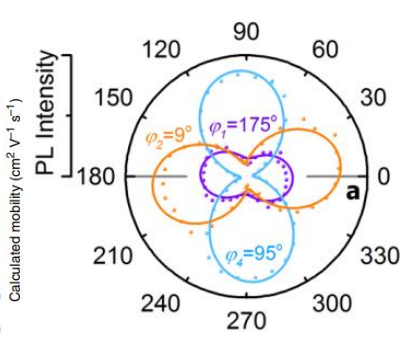
Structural anisotropy

Weak interlayer coupling



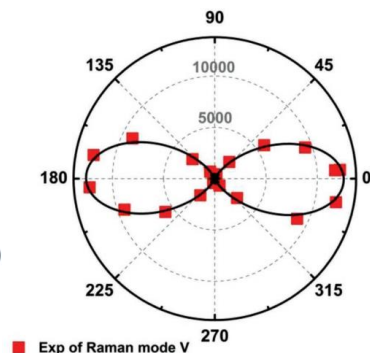
Electronic

*Nat. Commun.* **6**, 6991 (2015)



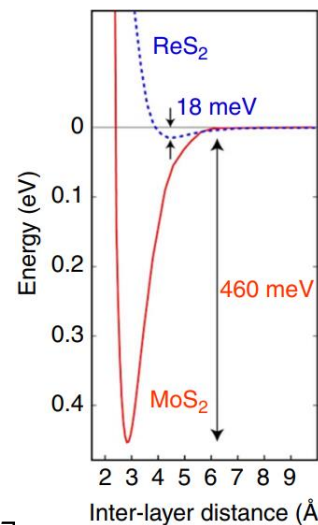
Optical

*Nano Lett.* **17**, 3202 (2017)

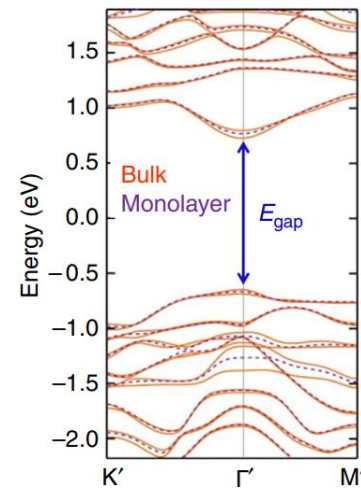


Vibrational

*Adv. Optical Mater.* **6**, 1800137 (2018)



Inter-layer distance (Å)

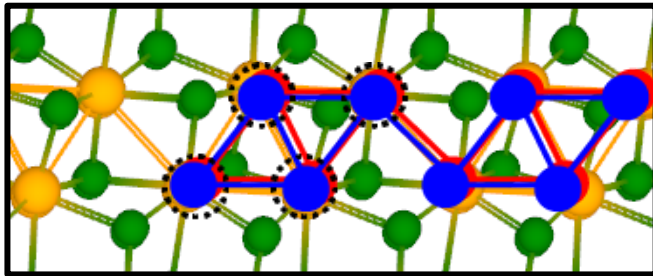
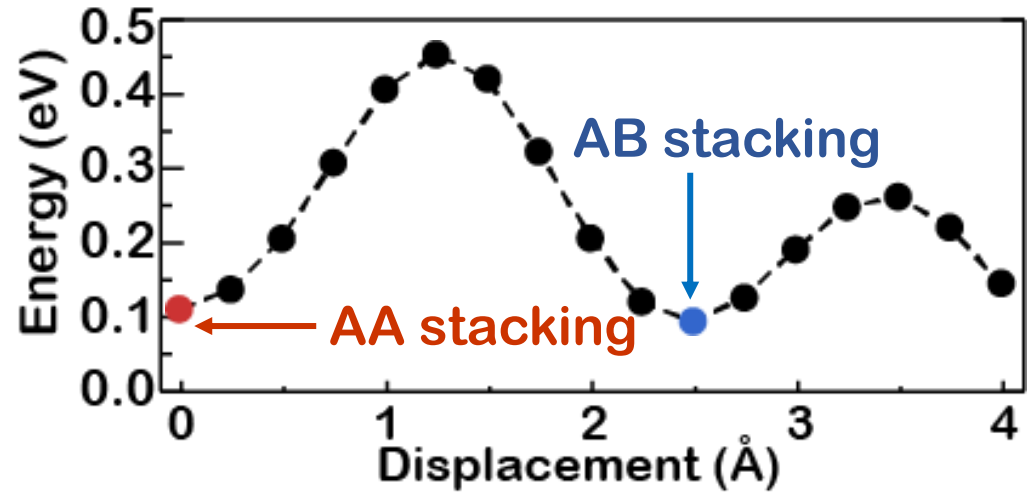
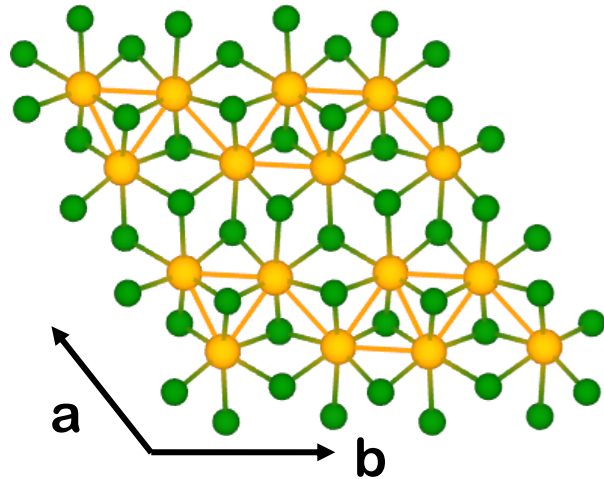


*Nat. Commun.* **5**, 3252 (2014)

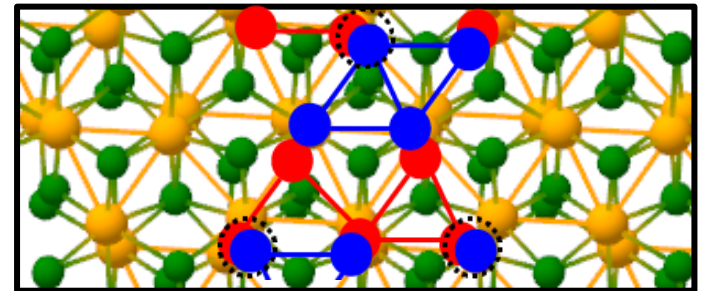
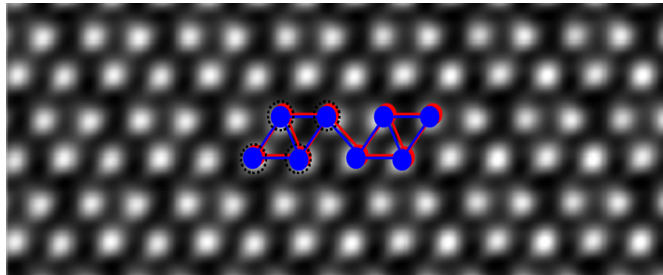
## Open challenges:

- Finding the stacking orders of multilayer ReS<sub>2</sub>

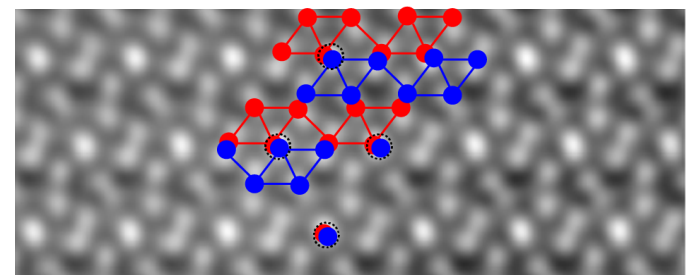
# Confirmation of stacking order



AA stacking

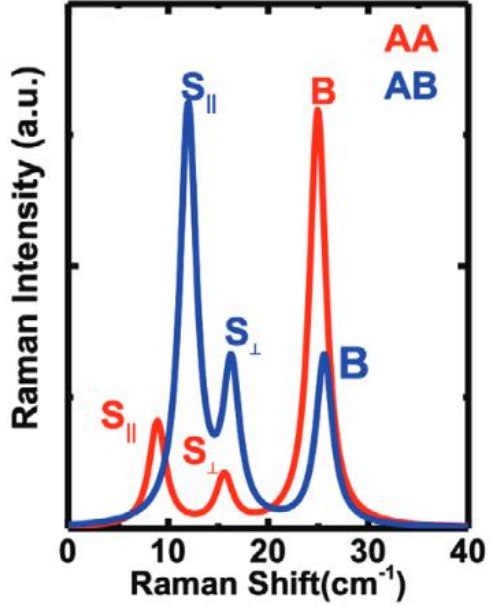
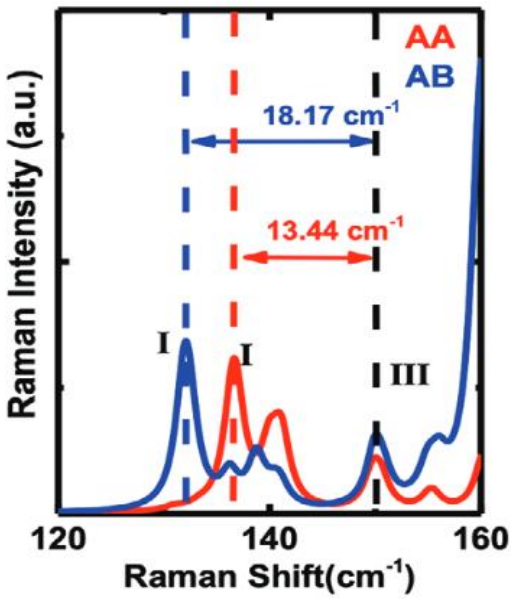


AB stacking

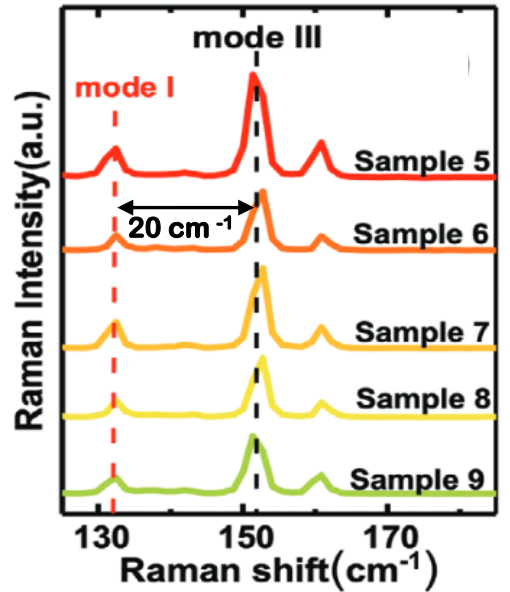
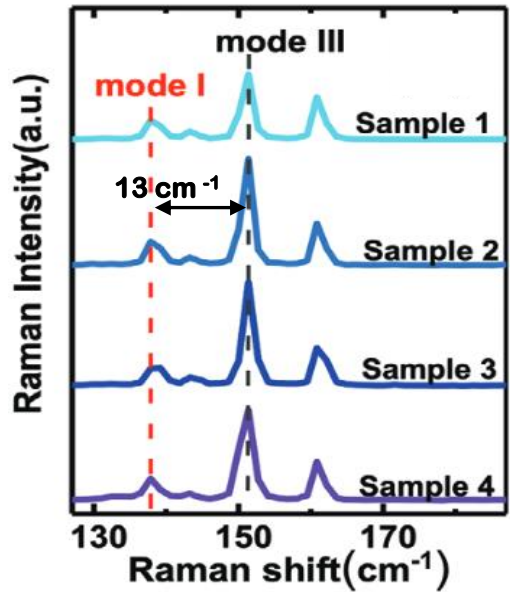


# Impact of stacking order

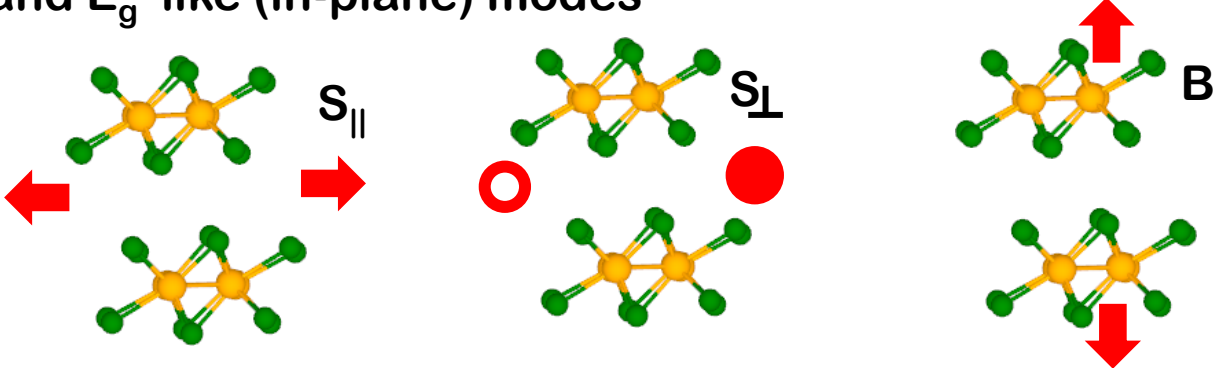
Theory



Experimental verification



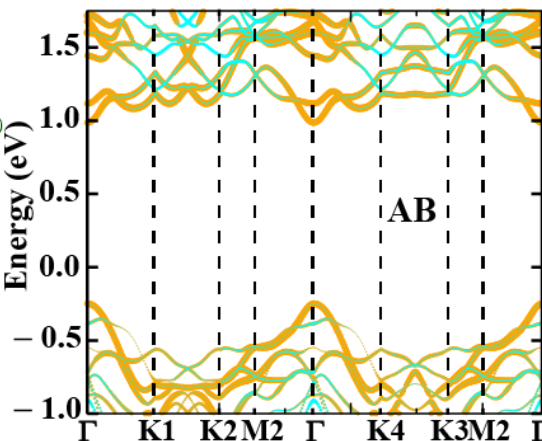
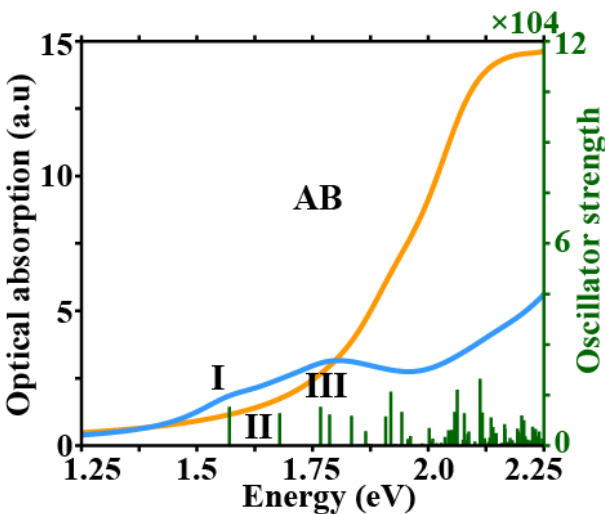
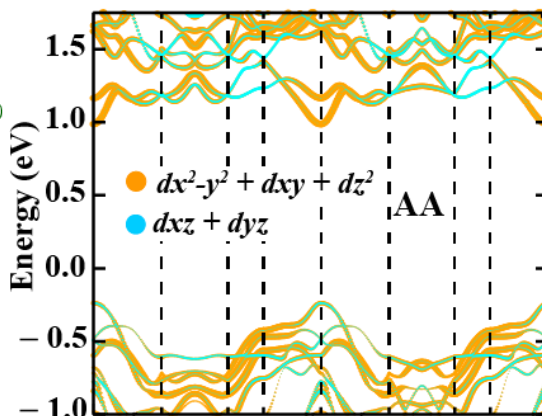
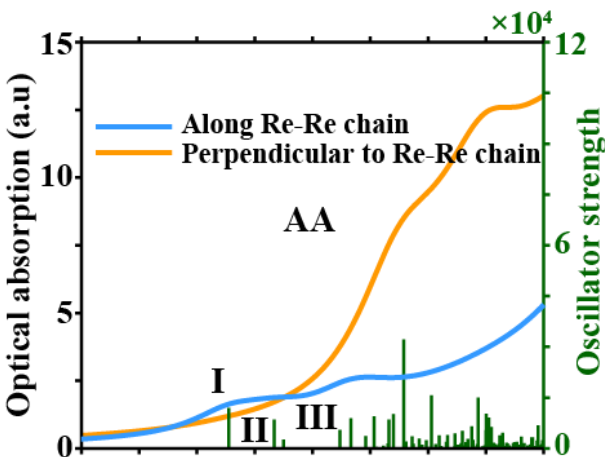
- Mode I and mode III correspond to the  $A_g^-$  (cross-plane) and  $E_g^-$  like (in-plane) modes



- Low-frequency breathing and shear modes indicate the stronger interlayer interaction in stacking AB

# Anisotropic optical properties

- The impact on the stacking order on optical properties in  $\text{ReS}_2$

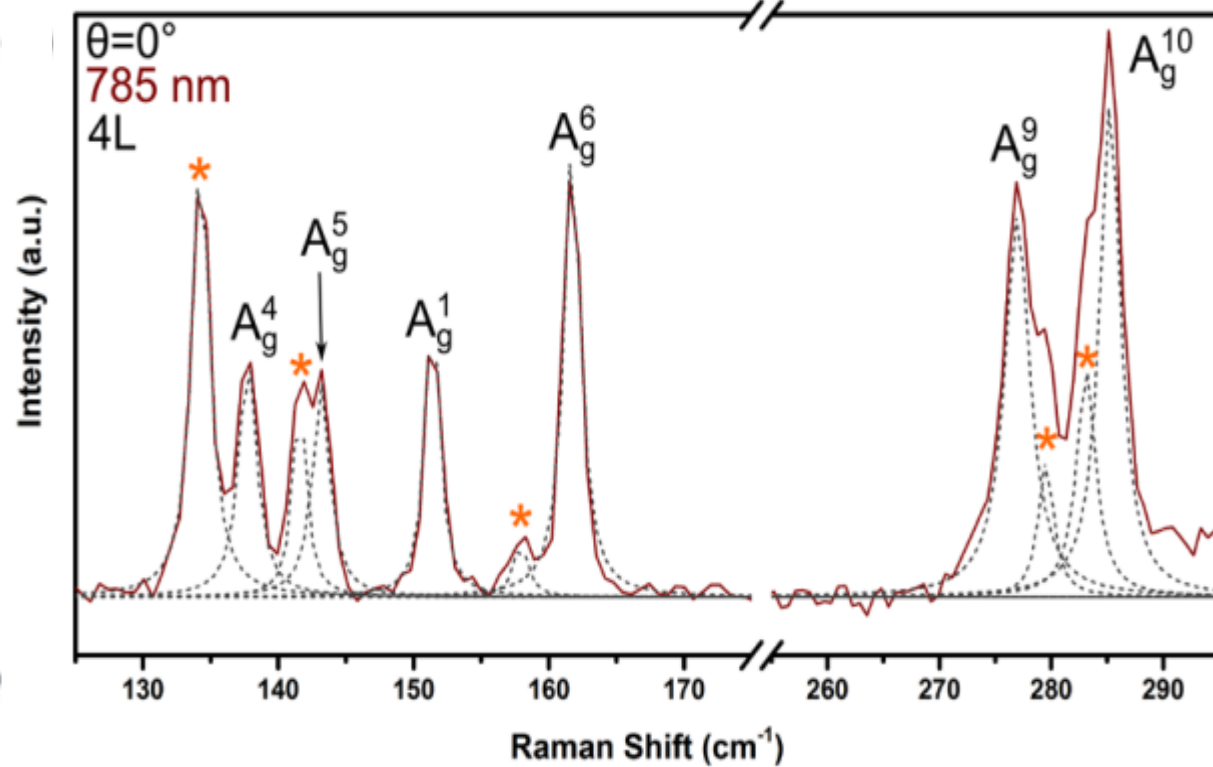
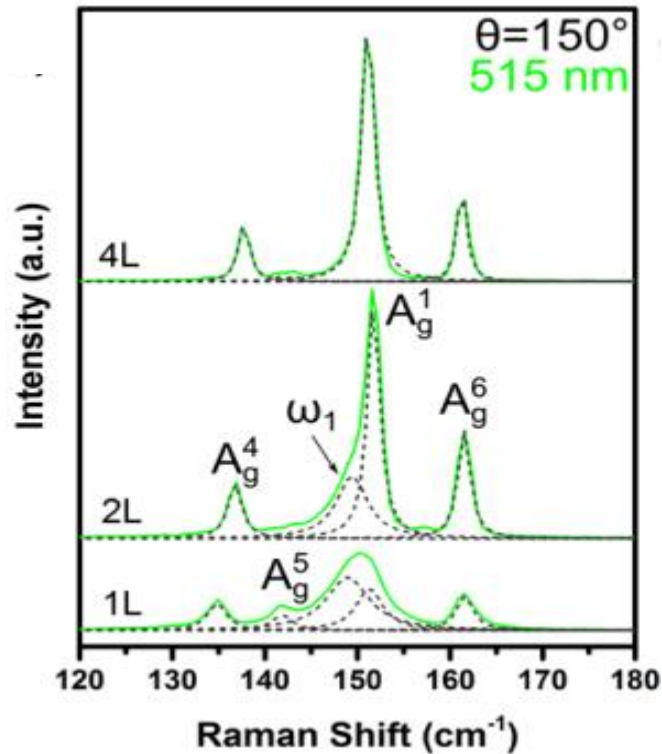


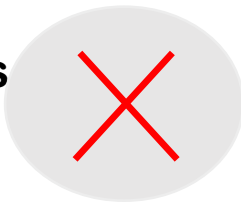
- Optical properties are more anisotropic in AB stacking
- Excitons are more delocalized in AB stacking
- Higher orbital contribution leads to increase the transition probability in AB stacking

- Exciton recombination faster in AB stacking

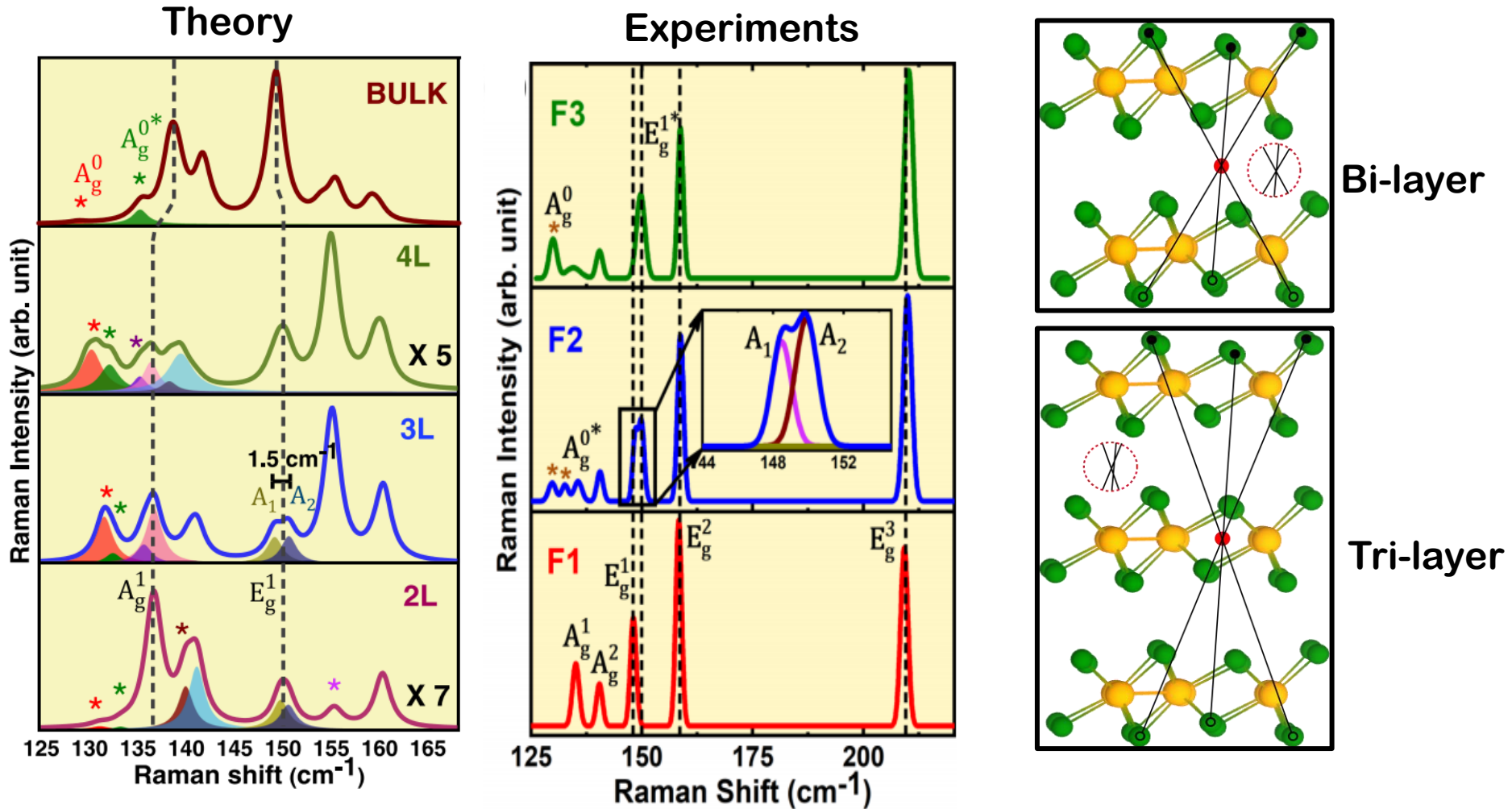


# Phonon modes splitting in multi-layers



- Previous literatures report
  - Defect activated IR modes 
  - Double resonance
- The HR-TEM and phonon calculations clear these doubts

# Layer parity dependent phonon modes



- Possible reasons

- Apparent changes in plane symmetry in 2L : Extra modes
- Breaking of inversion symmetry in 3L : Splitting modes

# Conclusions

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Two distinct stacking orders in ReS<sub>2</sub> are identified without ambiguity and resolve the conflict in the literature



Vibrational modes confirm the finite interlayer coupling strength



Optical properties (excitons) are more anisotropic and excitons are loosely bound in AB stacking than AA stacking



Deviation of crystal symmetry resolve the issues of stacking order dependency and extra ambiguous peaks in Raman spectra



# References:

1. Y. Zhou, **N. Maity**, A. Rai, R. Juneja, X. Meng, A. Roy, Y. Zhang, X. Xu, J. F. Lin, S. K. Banerjee, **A. K. Singh\***, and Y. Wang\*. **Adv. Mater. 32, 1908311 (2020) (Equal contribution)**
2. Y. Zhou, **N. Maity**, J. F. Lin, **A. K. Singh**, Y. Wang. **ACS Photonics 8, 405 (2021)**
3. P. Upadhyay, **N. Maity**, R. Kumar, P. K. Barman, **A. K. Singh\***, P. K. Nayak\*. **Phys. Rev. B 105, 045416 (2022) (Equal contribution)**

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- Mr. Yongjian Zhou, The University of Texas at Austin

## Computational facility

Materials Research Centre, IISc

SERC, IISc

TUE, IISc

# Thank You!