

# Investigations of 2D material metal contact using Density Functional Theory

**Anuja Chanana**

Nano Scale Device Research Laboratory

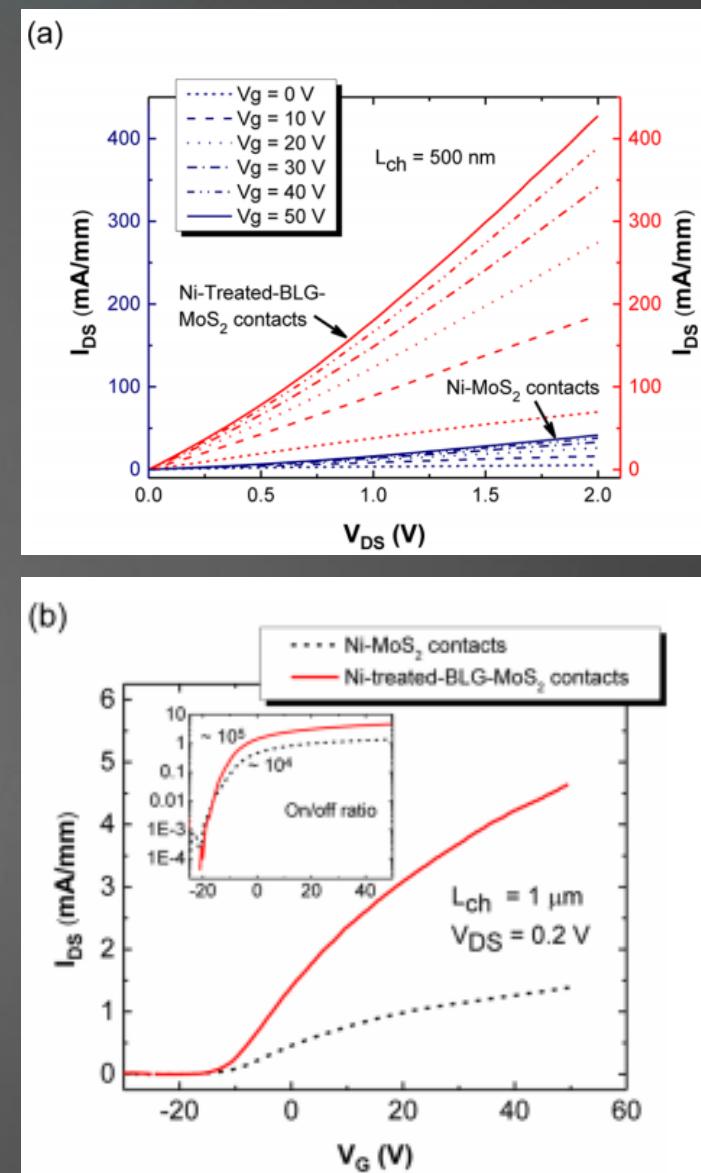
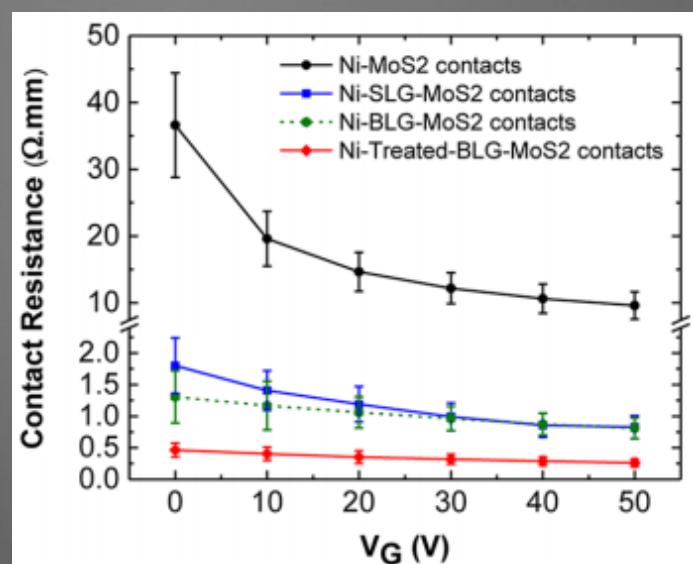
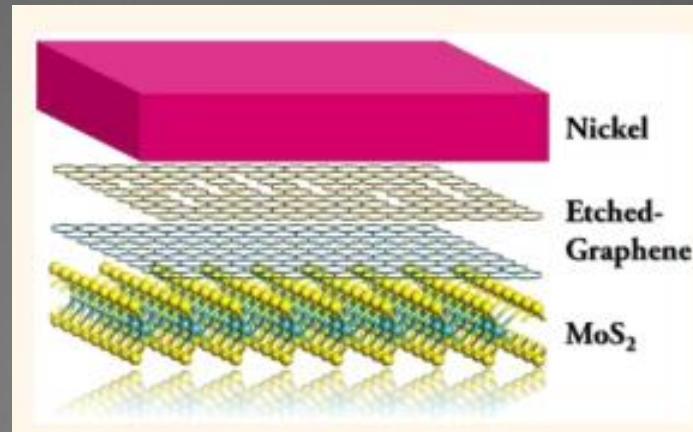
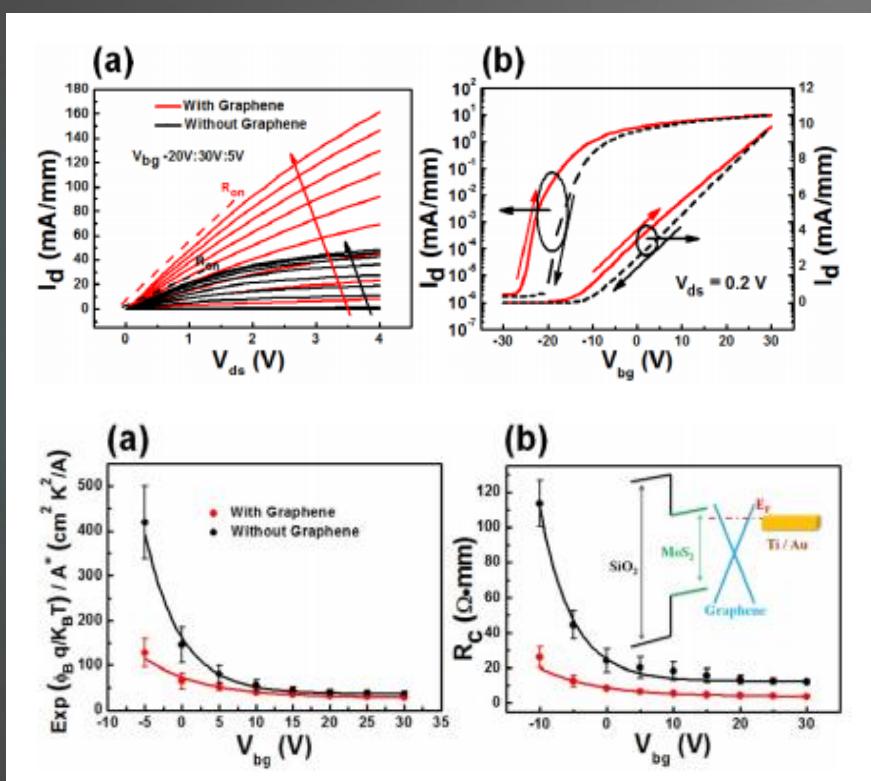
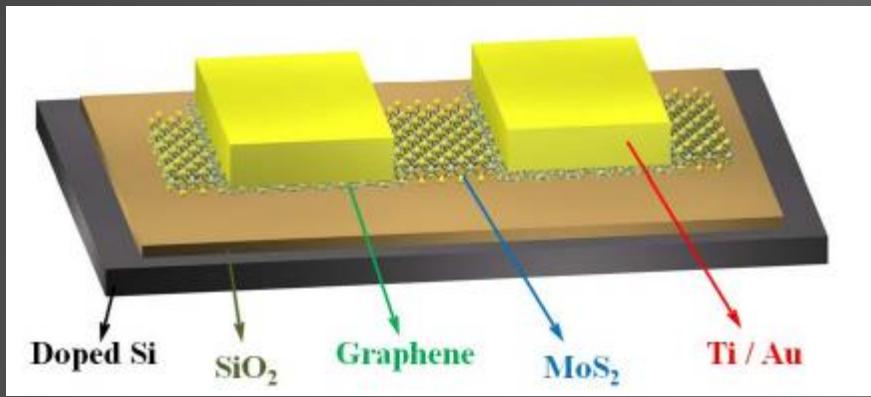
Research Supervisor

**Dr. Santanu Mahapatra**

# SBH MODIFICATION USING GRAPHENE INSERTED MoS<sub>2</sub>-METAL CONTACT

- ❖ Experimental reports
- ❖ Interface geometry
- ❖ Computational challenges
- ❖ SBH evaluation
- ❖ Orbital hybridization
- ❖ Work Function calculation
- ❖ Fermi level pinning

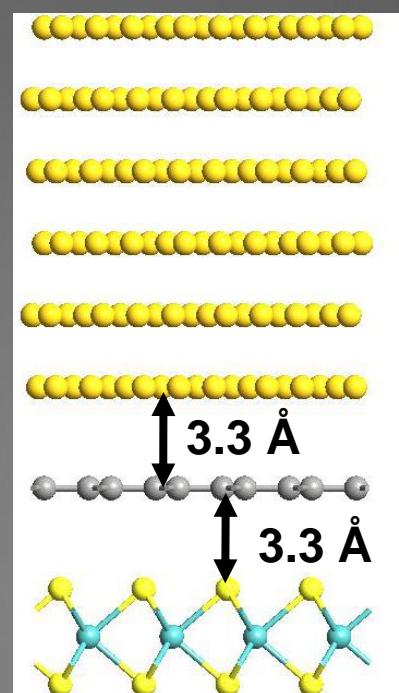
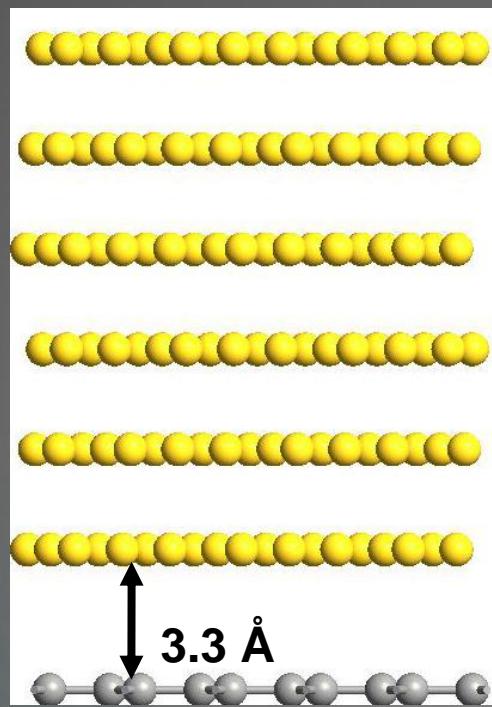
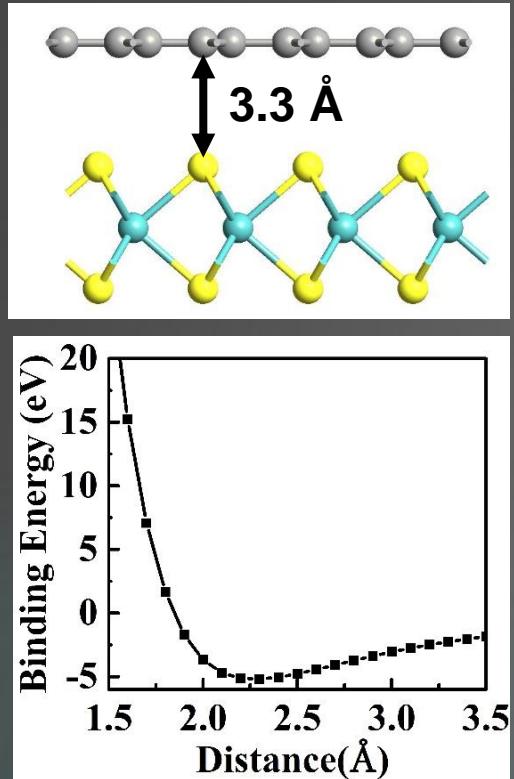
# EXPERIMENTAL REPORTS



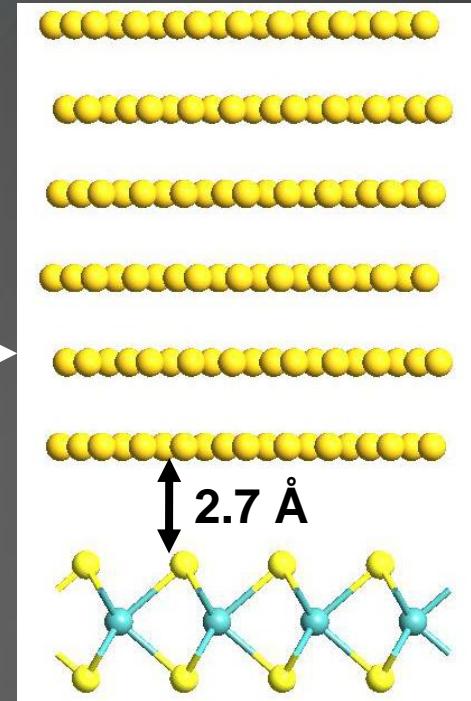
Ref. Du et. al IEEE EDL, VOL. 35, NO. 5, MAY 2014

Ref. Leong et.al ACS Nano, 2015, 9 (1), pp 869–877

# INTERFACE GEOMETRY (1 of 2)

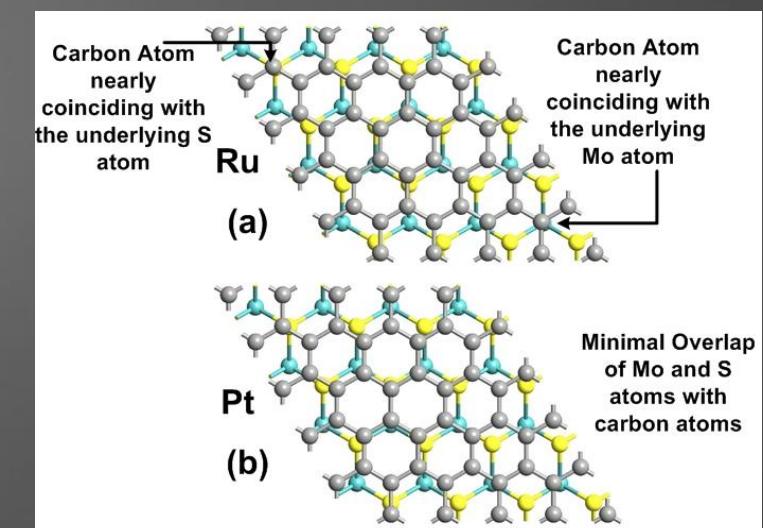
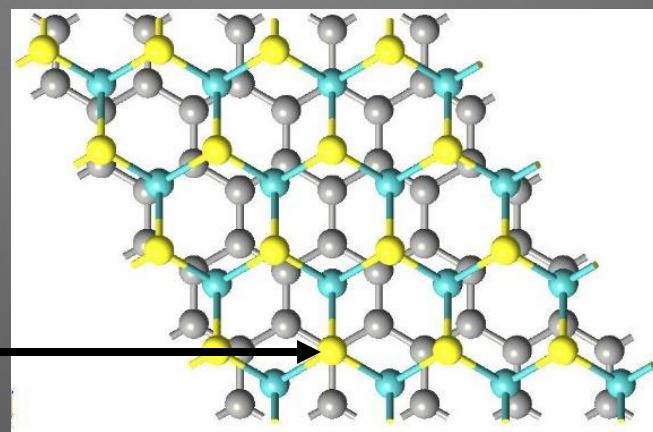


Comparison

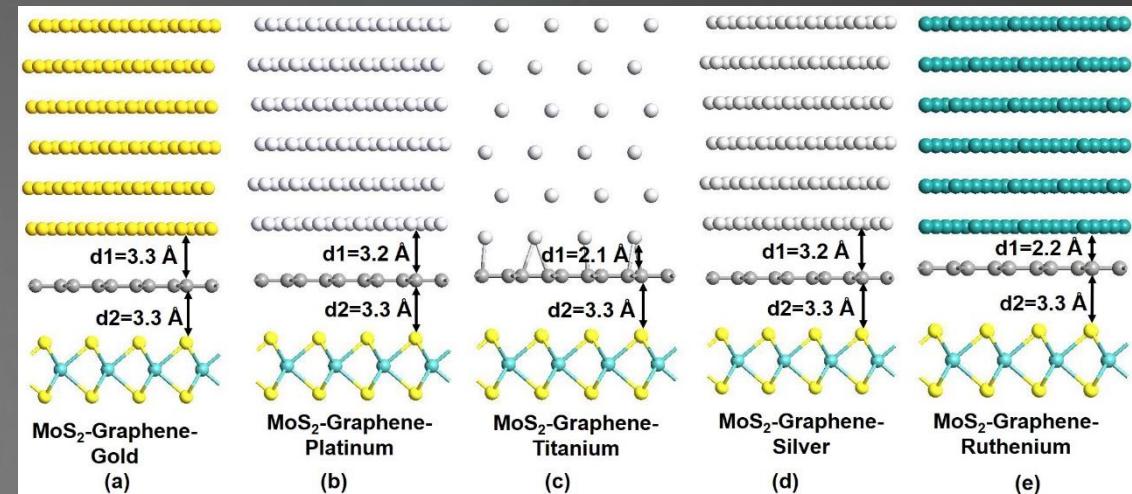
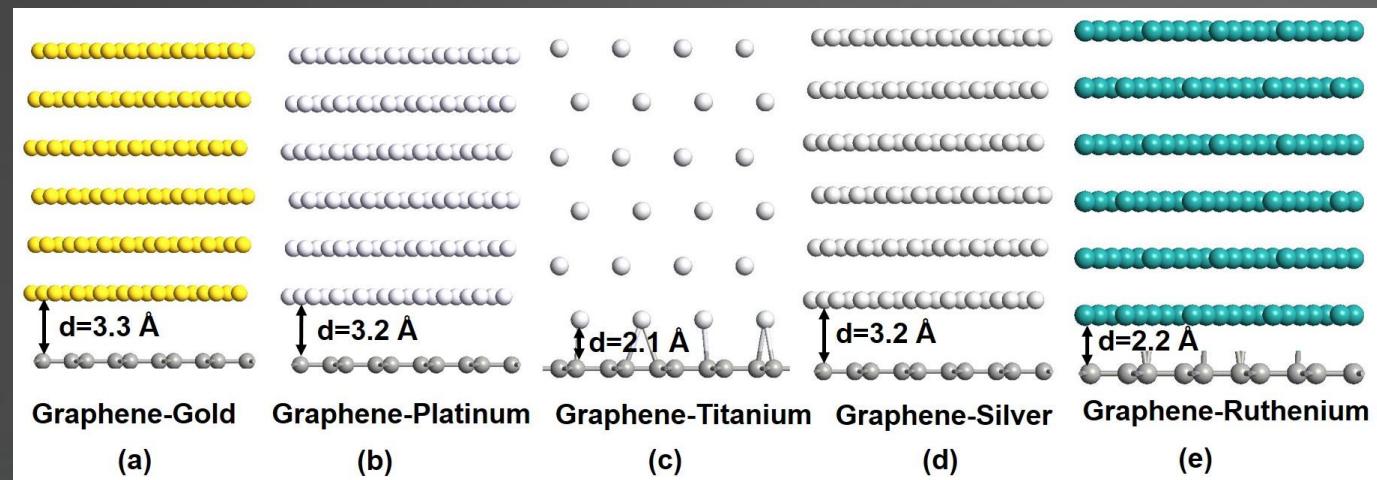


$$\text{Binding Energy} = \text{Total Energy (A+B)} - \text{Total Energy (A)} - \text{Total Energy (B)}$$

C atom coinciding with S atom (TS)



# INTERFACE GEOMETRY (2 of 2)



System	MoS <sub>2</sub> -G	G-Au	G-Pt	G-Ti	G-Ag	G-Ru	MoS <sub>2</sub> -Au	MoS <sub>2</sub> -Pt	MoS <sub>2</sub> -Ti	MoS <sub>2</sub> -Ag	MoS <sub>2</sub> -Ru	MoS <sub>2</sub> -G-Au	MoS <sub>2</sub> -G-Pt	MoS <sub>2</sub> -G-Ti	MoS <sub>2</sub> -G-Ag	MoS <sub>2</sub> -G-Ru
Strain(%)	1.8	1.8	1.2	2.8	1.5	0.5	0.38	0.38	1.1	0.26	1.3	1.8	1.8	1.8	1.8	1.8
d(Å)	3.3	3.3	3.2	2.1	3.2	2.2	2.7	2.3	2.2	2.5	2.2	d1=3.3 d2=3.3	d1=3.3 d2=3.2	d1=3.3 d2=2.1	d1=3.3 d2=3.2	d1=3.3 d2=2.2
BE(eV)	-1.86	-2.5	-3	-19	-2.15	-5	-5.9	-9.55	-17.5	-6.5	-14.8	-4.5	-5.16	-23.81	-4.3	-12.43

# COMPUTATIONAL CHALLENGES

- ❖ Interface Relaxation
- ❖ Fritz-Haber-Institute (FHI) versus Hartwingster-Goedecker-Hutter (HGH) - Gold

Single Zeta 5d 6s  
Double Zeta 5d 6s 5d 6s  
Single Zeta Polarized 5d 6s 7p  
Double Zeta Polarized 5d 6s 5d 6s 7p

Double Zeta Double Polarized 5d 6s 5d 6s 7p 7p

- ❖ Machine specifications

Machine 1

Number of CPUS's 24

Memory 256 GB

Machine 2

Number of CPUS's 20

Memory 386 GB

- ❖ Palladium Tier 8 4s 4p 4d 5s 5p 4d 4f 5p 5s 4d 4d

- ❖ MoS<sub>2</sub>-Graphene-Gold 228148.05 s (2d15h22m28.05s)

- ❖ MoS<sub>2</sub>-Graphene-Ruthenium 304372.35 s (3d12h32m52.35s)

versus

Hartwingster-Goedecker-Hutter (HGH) - Gold

Tier 0 5d 6s

Tier 1 5d 6s 6p

Tier 2 5d 6s 6p 6s

Tier 3 5d 6s 6p 6s 6d

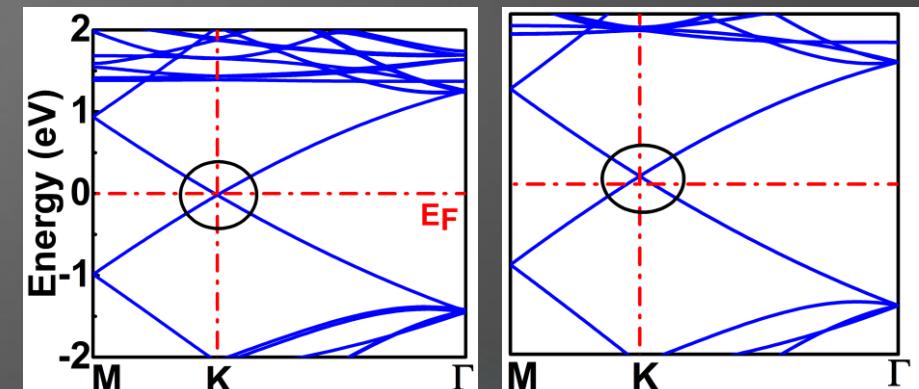
Tier 4 5d 6s 6p 6s 6d 6s

Tier 5 5d 6s 6p 6s 6d 6s 6d

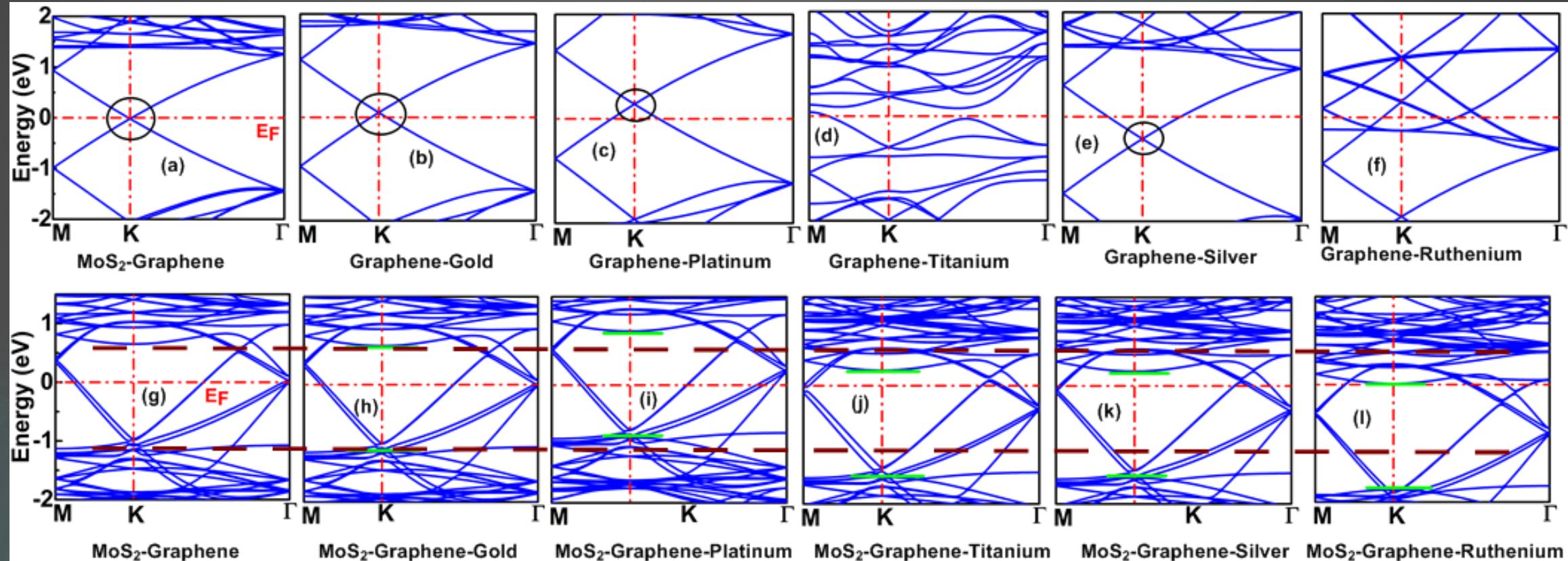
Tier 6 5d 6s 6p 6s 6d 6s 6d 5f

Tier 7 5d 6s 6p 6s 6d 6s 6d 5f 6p

Tier 8 5d 6s 6p 6s 6d 6s 6d 5f 6p 6f

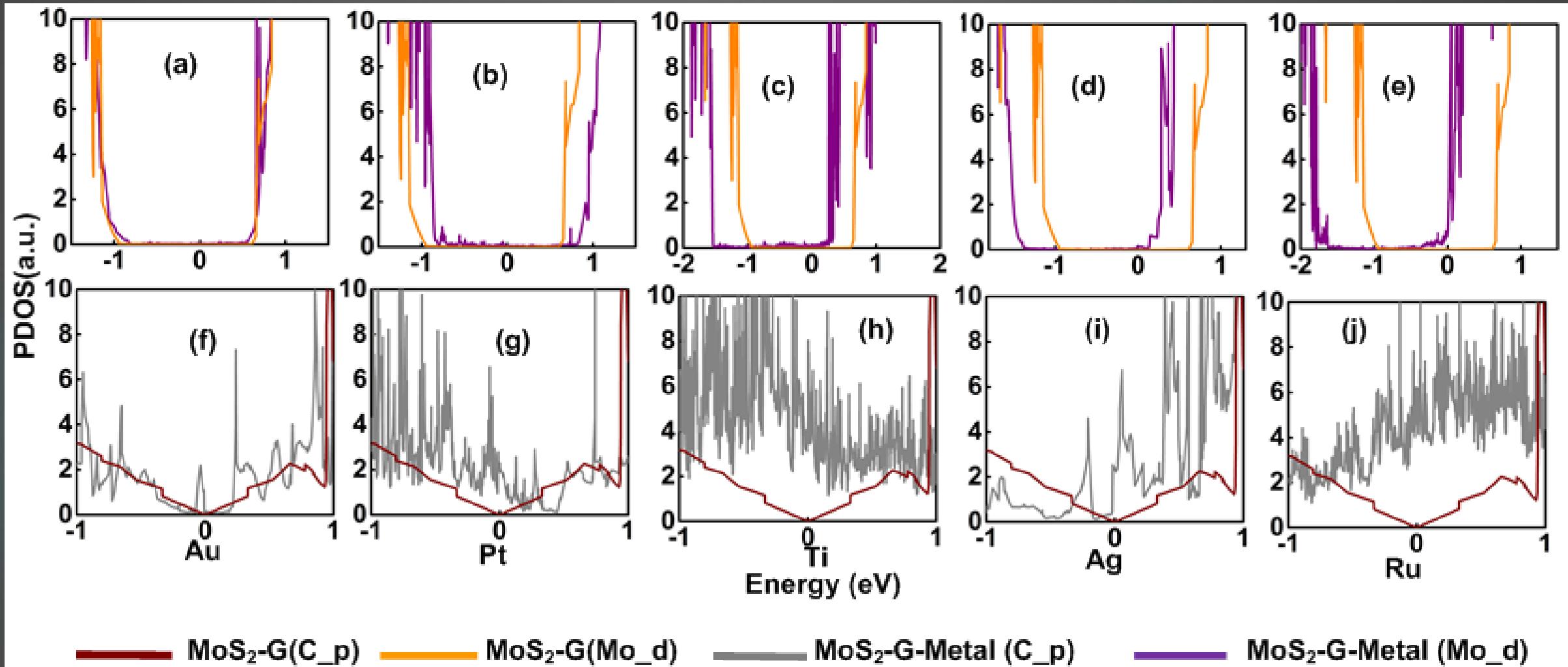


# SBH EVALUATION



System	MoS <sub>2</sub> -G	G-Au	G-Pt	G-Ti	G-Ag	G-Ru	MoS <sub>2</sub> -Au	MoS <sub>2</sub> -Pt	MoS <sub>2</sub> -Ti	MoS <sub>2</sub> -Ag	MoS <sub>2</sub> -Ru	MoS <sub>2</sub> -G-Au	MoS <sub>2</sub> -G-Pt	MoS <sub>2</sub> -G-Ti	MoS <sub>2</sub> -G-Ag	MoS <sub>2</sub> -G-Ru
$\Delta E_F$	-0.02	0.1	0.28	—	-0.423	—	—	—	—	—	—	-0.106	0.127	—	-0.057	—
n-SBH	0.65	—	—	—	—	—	0.64	0.81	0.382	0.373	0.56	0.663	0.916	0.26	0.25	0.018
p-SBH	1.14	—	—	—	—	—	1.2	1.09	1.67	1.48	1.34	1.14	0.89	1.55	1.56	1.79
$E_g$ (eV)	1.79	—	—	—	—	—	1.84	1.9	2.052	1.853	1.9	1.803	1.806	1.81	1.81	1.808

# ORBITAL HYBRIDIZATION



# CHARGE REDISTRIBUTION

$$\Delta\rho = \rho_{MoS_2+graphene+metal} - \rho_{MoS_2} - \rho_{graphene} - \rho_{metal}$$

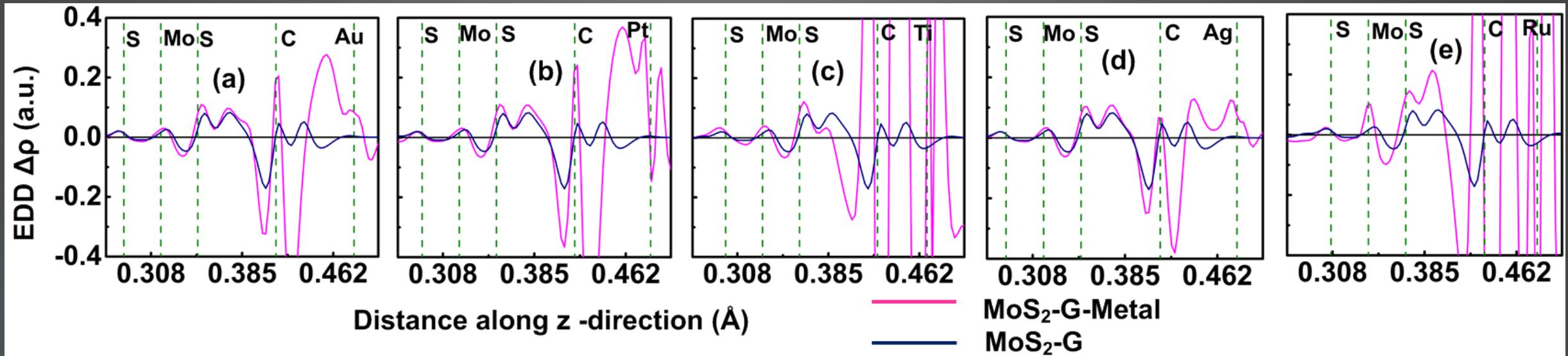
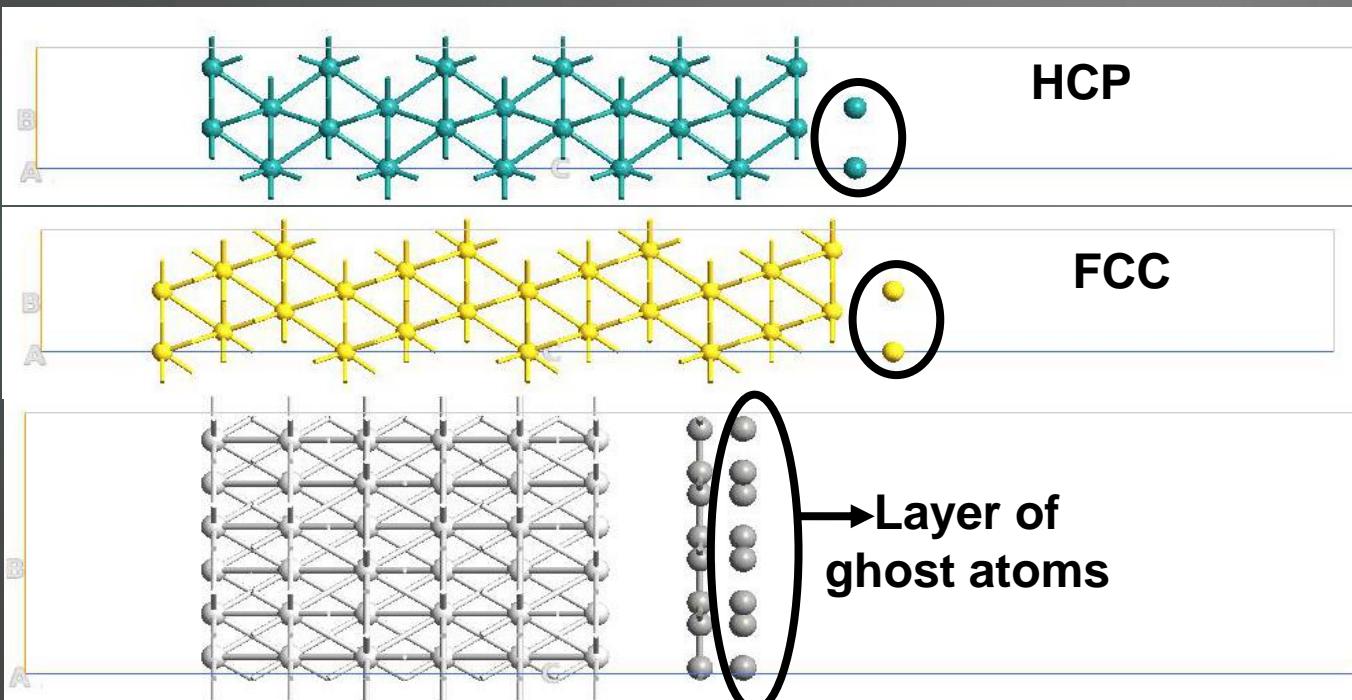
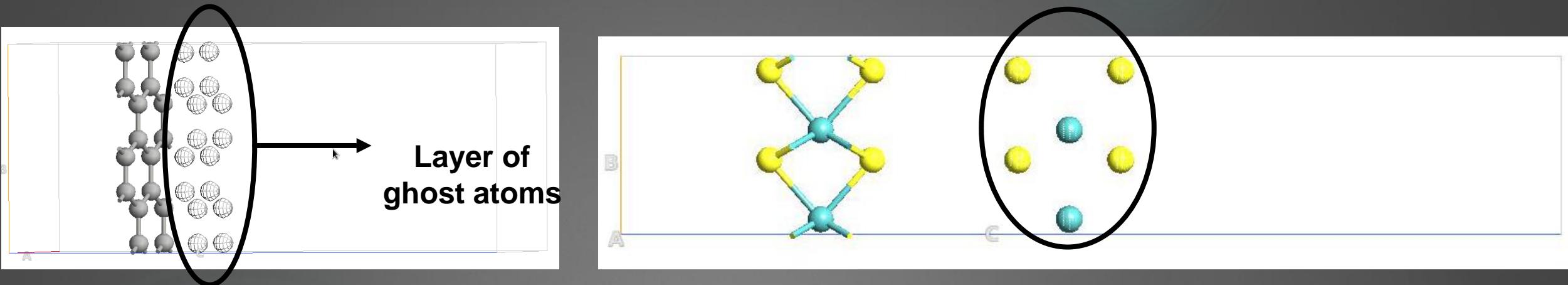


TABLE II: Area calculated between the interfacial sulfur atom of MoS<sub>2</sub> and carbon atom of graphene for various MoS<sub>2</sub>-graphene-metal interface.

System	Area Under EDD between C and S atoms
MoS <sub>2</sub> -G	$1.7 \times 10^{-7}$
MoS <sub>2</sub> -G-Au	$-1.04 \times 10^{-7}$
MoS <sub>2</sub> -G-Ag	$3.42 \times 10^{-7}$
MoS <sub>2</sub> -G-Ti	$5.62 \times 10^{-6}$
MoS <sub>2</sub> -G-Pt	$-3 \times 10^{-7}$
MoS <sub>2</sub> -G-Ru	$8.1 \times 10^{-6}$

# WORK FUNCTION CALCULATION

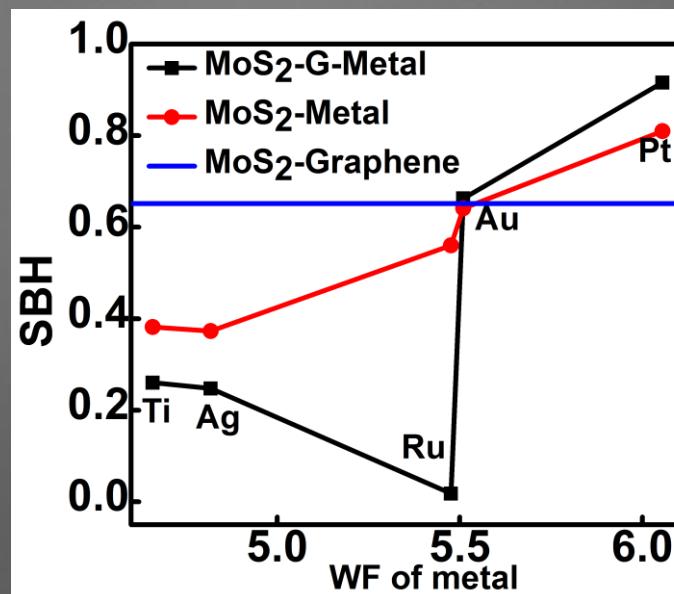
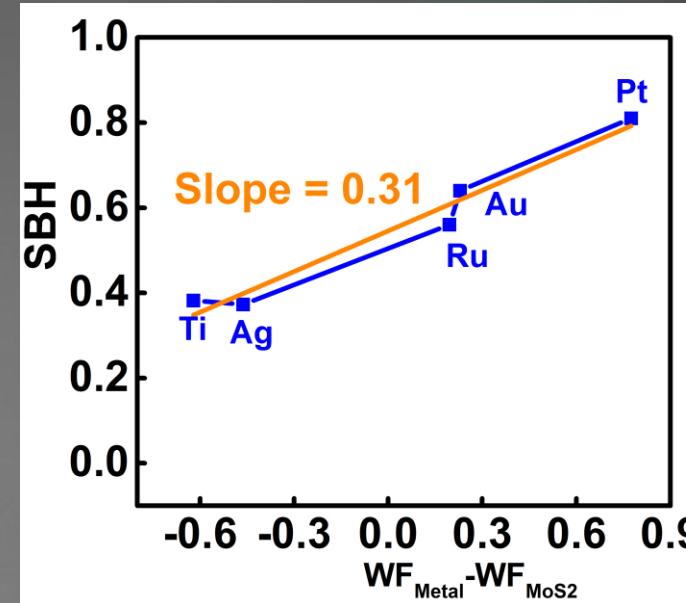
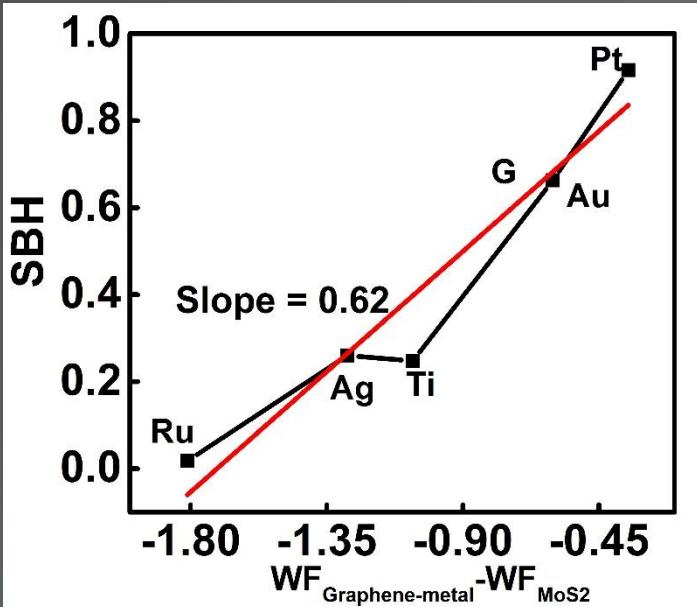


Metal	Calculated	Reported
Titanium	4.6589	4.56
Silver	4.81793	4.74
Ruthenium	5.47582	5.14
Gold	5.50947	5.54
Platinum	6.05502	6.13

Ref. P. A. Khomyakov et.al PHYSICAL REVIEW B 79, 195425 2009

Ref. Cheng Gong J. Appl. Phys. 108, 123711 2010

# FERMI LEVEL PINNING



# CONCLUSION

- ❖ We address the reduction n-SBH by inserting graphene layer between  $\text{MoS}_2$  and metal contact for five different metals (Au, Ti, Ag, Pt and Ru).
- ❖ A decrease in SBH is not consistent among various metals, rather an increase in SBH is observed in case of Au and Pt .
- ❖ Unlike  $\text{MoS}_2$ -metal interface, the projected dispersion of  $\text{MoS}_2$  remains preserved in any  $\text{MoS}_2$ -graphene-metal system with shift in the bands on the energy axis.
- ❖ A proper choice of metal (e.g., Ru) may exhibit Ohmic nature in a graphene inserted  $\text{MoS}_2$ -metal contact.
- ❖ These understandings would provide a direction in developing high performance transistors involving hetero atomic layers as contact electrodes.

# QUESTIONS??