

Investigations of 2D material metal contact using Density Functional Theory

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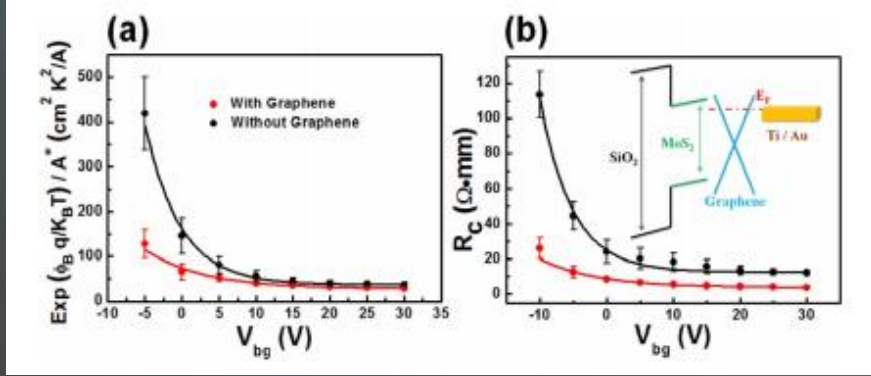
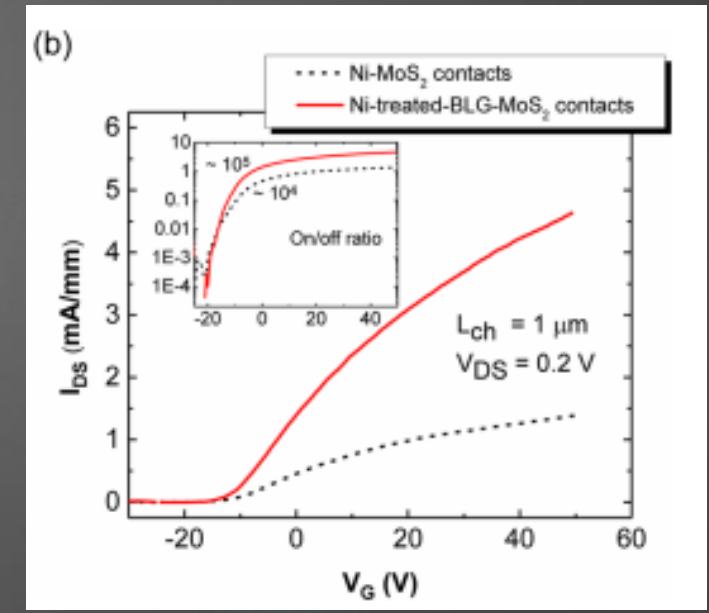
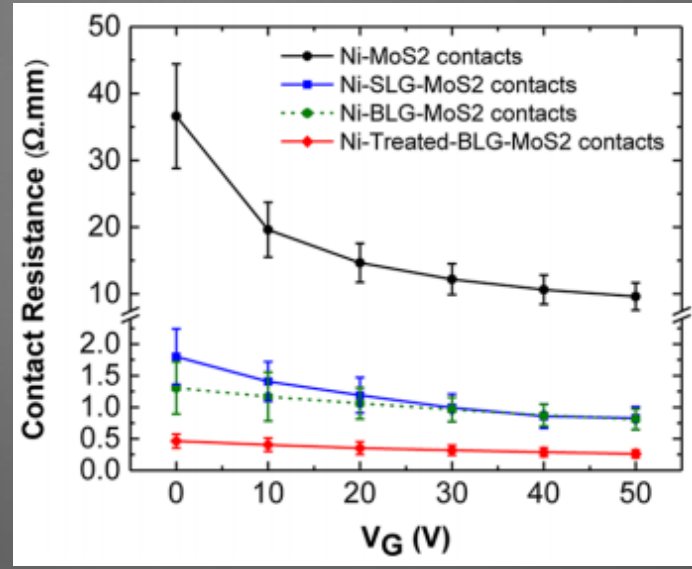
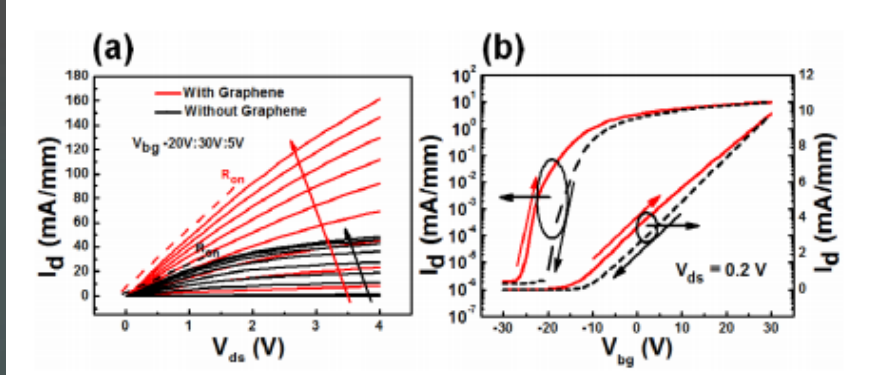
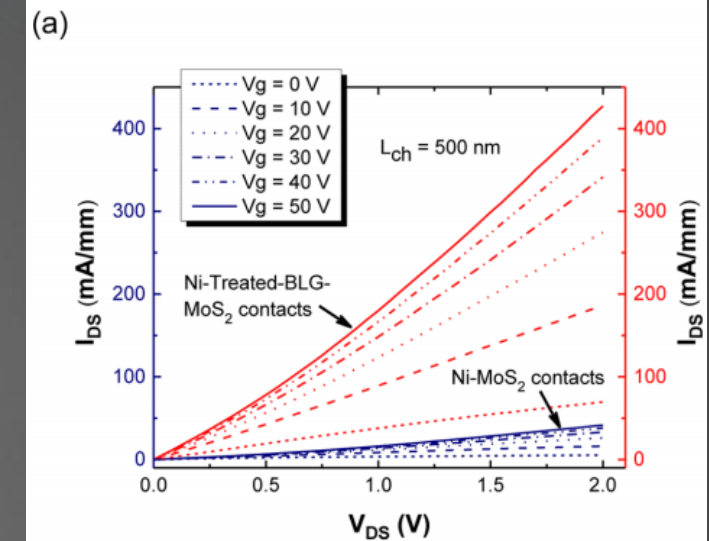
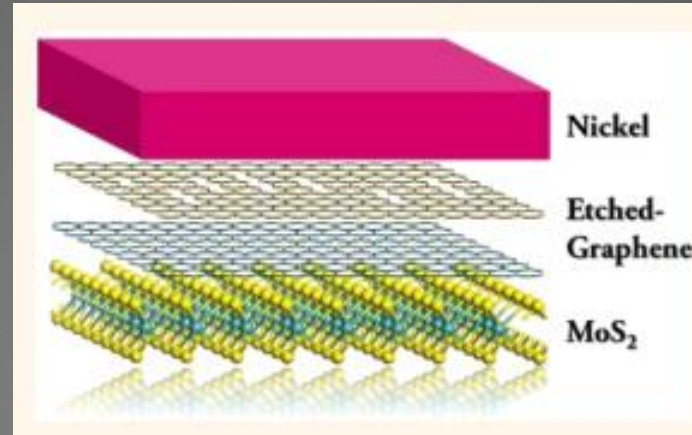
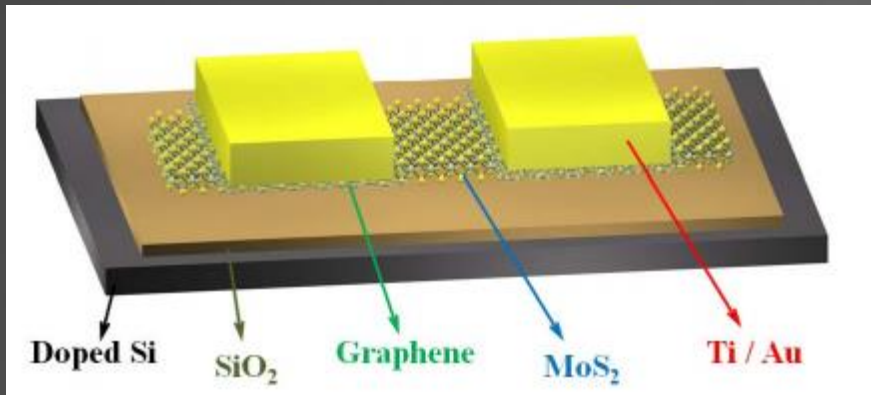
Research Supervisor

Dr. Santanu Mahapatra

SBH MODIFICATION USING GRAPHENE INSERTED MoS₂-METAL CONTACT

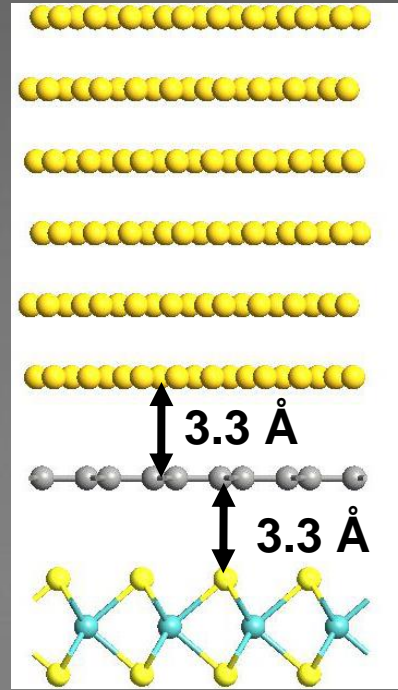
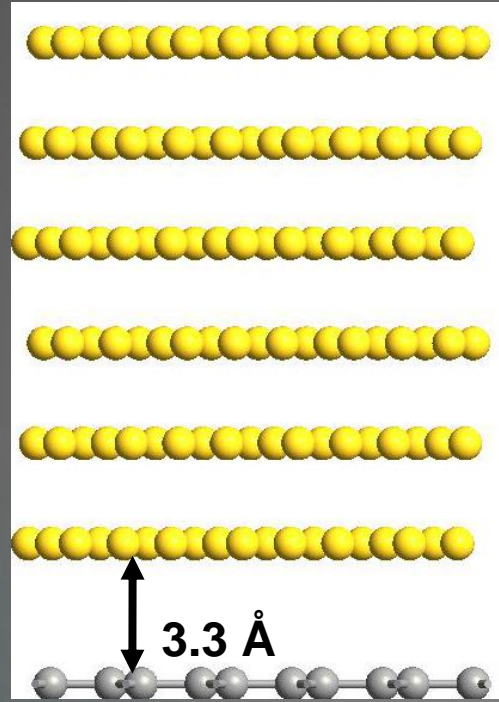
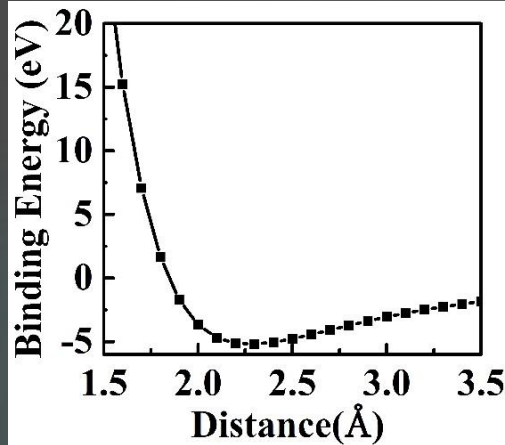
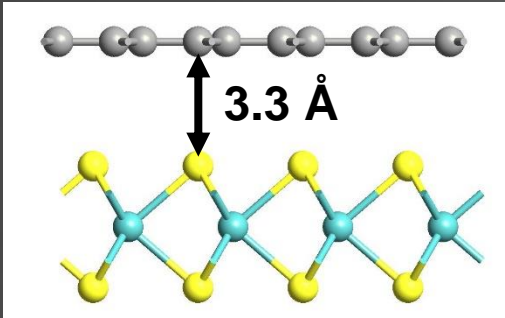
- ❖ Experimental reports
- ❖ Interface geometry
- ❖ Computational challenges
- ❖ SBH evaluation
- ❖ Orbital hybridization
- ❖ Work Function calculation
- ❖ Fermi level pinning

EXPERIMENTAL REPORTS

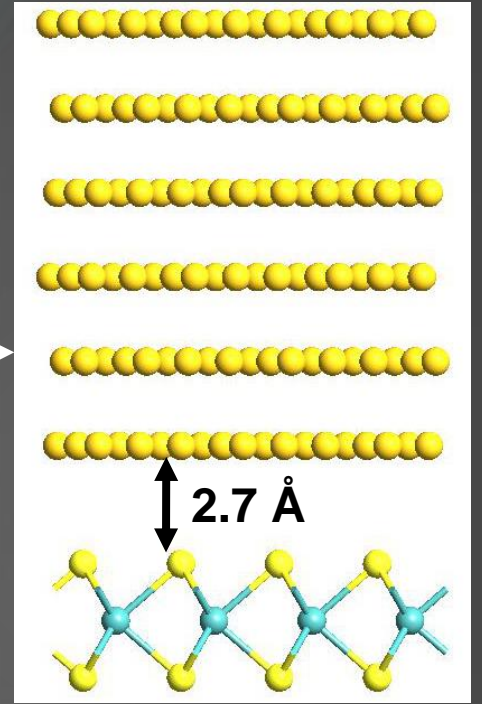


Ref. Du et. al IEEE EDL, VOL. 35, NO. 5, MAY 2014
 Ref. Leong et.al ACS Nano, 2015, 9 (1), pp 869–877

INTERFACE GEOMETRY (1 of 2)

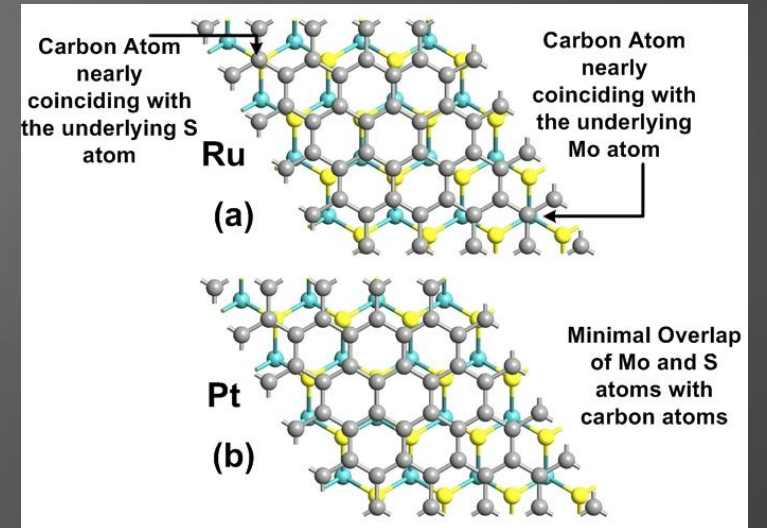
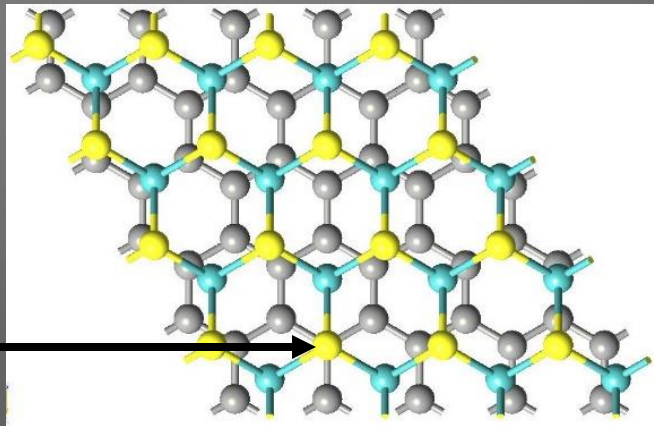


Comparison

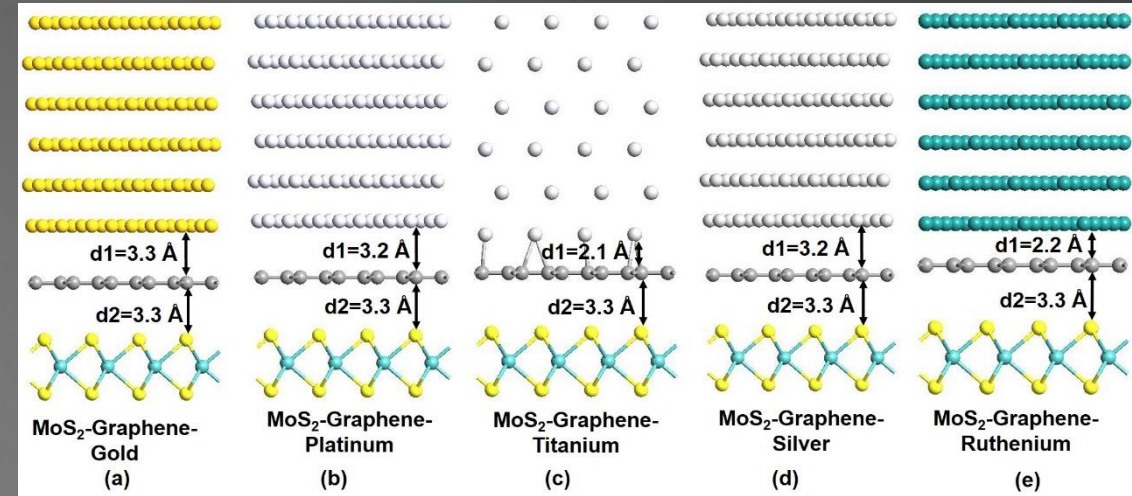
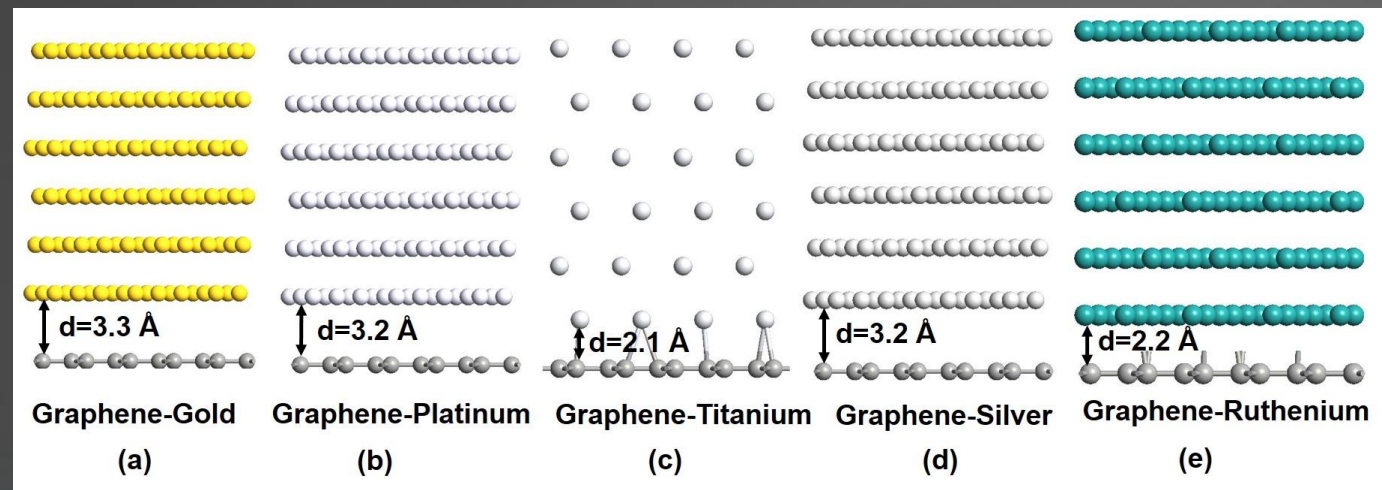


$$\text{Binding Energy} = \text{Total Energy (A+B)} - \text{Total Energy (A)} - \text{Total Energy (B)}$$

C atom coinciding with S atom (TS)



INTERFACE GEOMETRY (2 of 2)



System	MoS ₂ -G	G-Au	G-Pt	G-Ti	G-Ag	G-Ru	MoS ₂ -Au	MoS ₂ -Pt	MoS ₂ -Ti	MoS ₂ -Ag	MoS ₂ -Ru	MoS ₂ -G-Au	MoS ₂ -G-Pt	MoS ₂ -G-Ti	MoS ₂ -G-Ag	MoS ₂ -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

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

❖ Machine specifications

Machine 1

Machine 2

Number of CPUs's 24

Number of CPUs's 20

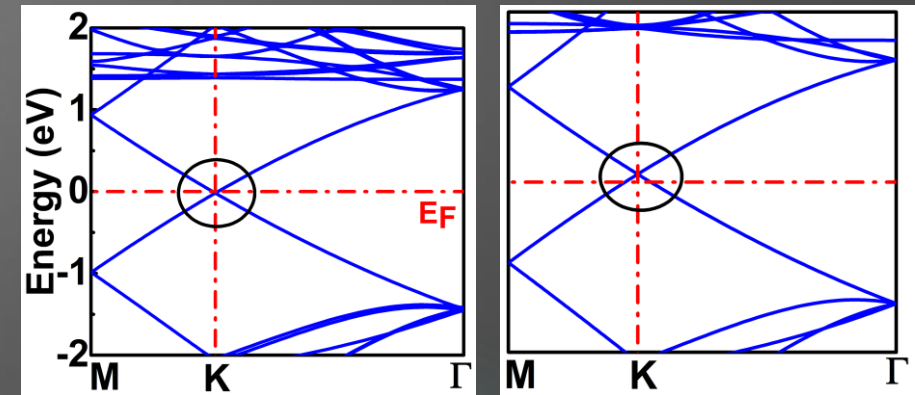
Memory 256 GB

Memory 386 GB

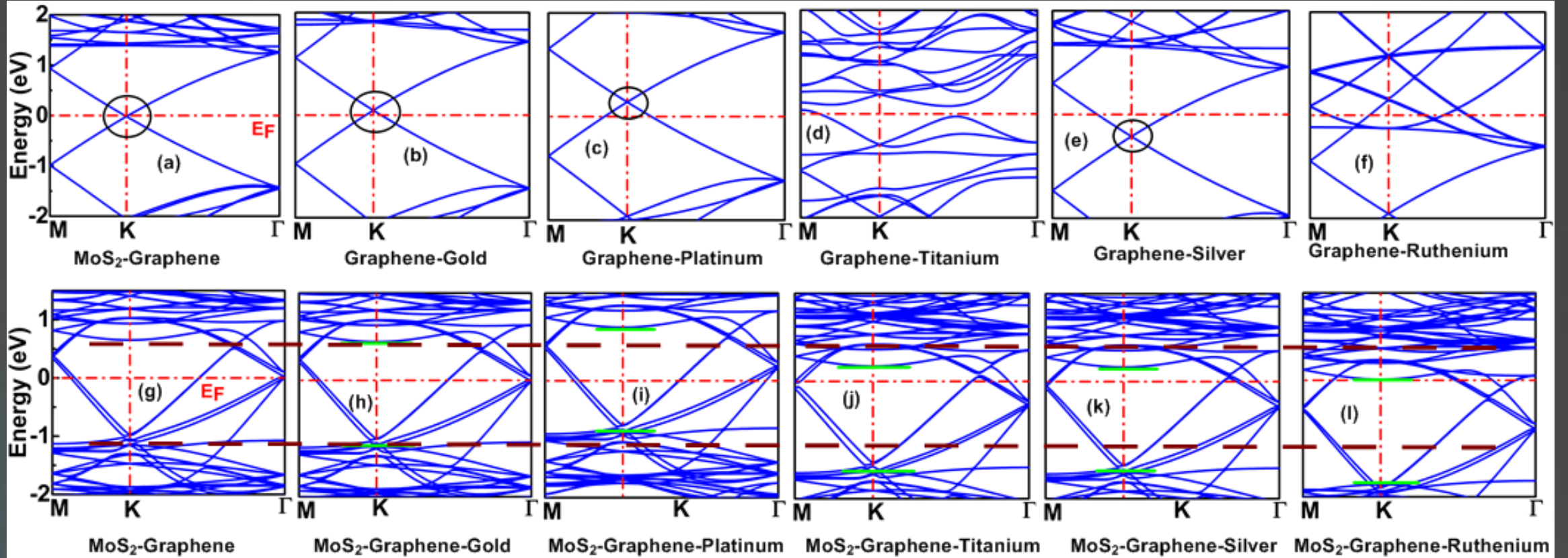
❖ Palladium Tier 8 4s 4p 4d 5s 5s 5p 4d 4f 5p 5s 4d 4d

❖ MoS₂-Graphene-Gold 228148.05 s (2d15h22m28.05s)

❖ MoS₂-Graphene-Ruthenium 304372.35 s (3d12h32m52.35s)

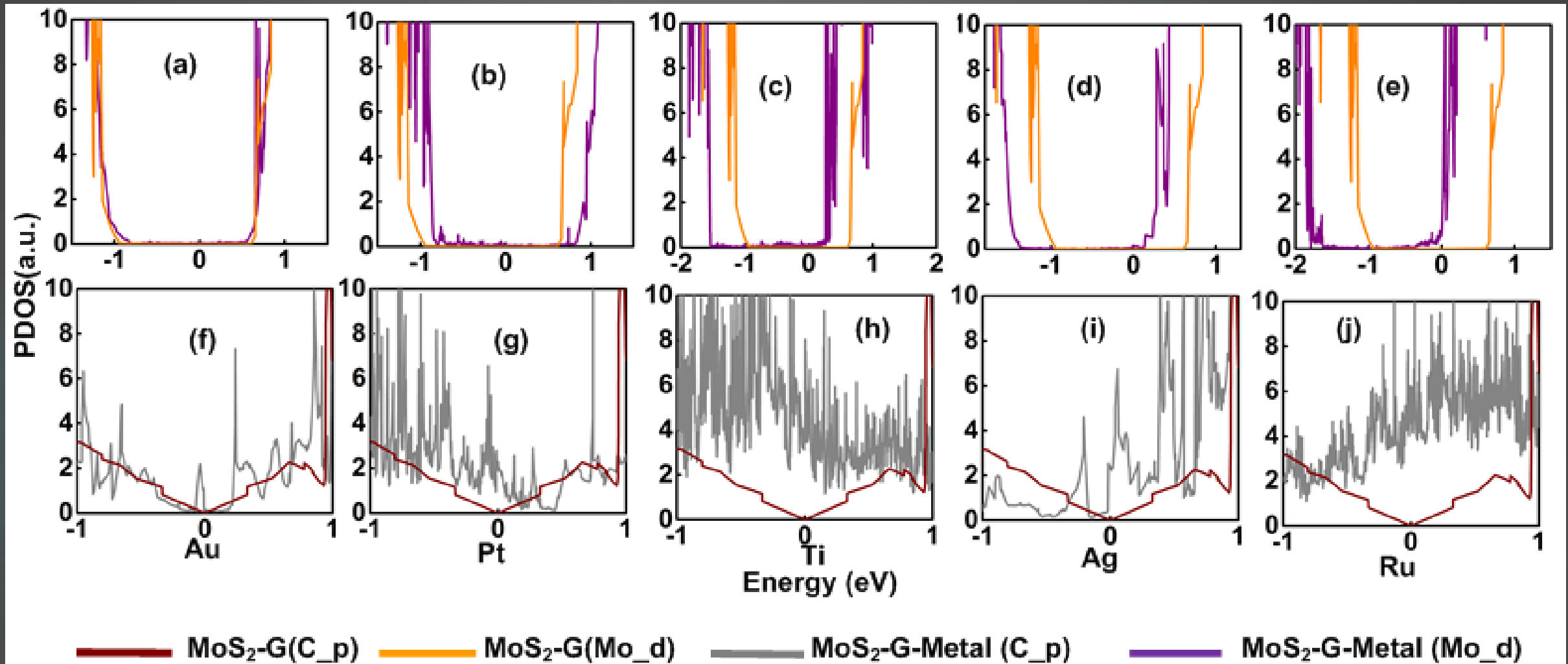


SBH EVALUATION



System	MoS ₂ - G	MoS ₂ - G-Au	MoS ₂ - G-Pt	MoS ₂ - G-Ti	MoS ₂ - G-Ag	MoS ₂ - G-Ru	MoS ₂ - Au	MoS ₂ - Pt	MoS ₂ - Ti	MoS ₂ - Ag	MoS ₂ - Ru	MoS ₂ - G-Au	MoS ₂ - G-Pt	MoS ₂ - G-Ti	MoS ₂ - G-Ag	MoS ₂ - G-Ru
ΔE_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

$$\Delta\rho = \rho_{\text{MoS}_2+\text{graphene}+\text{metal}} - \rho_{\text{MoS}_2} - \rho_{\text{graphene}} - \rho_{\text{metal}}$$

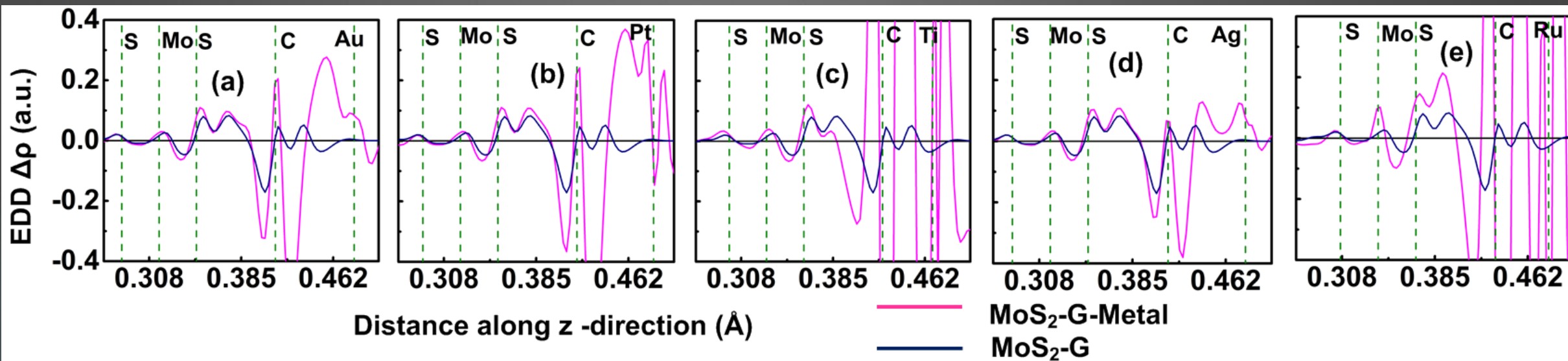
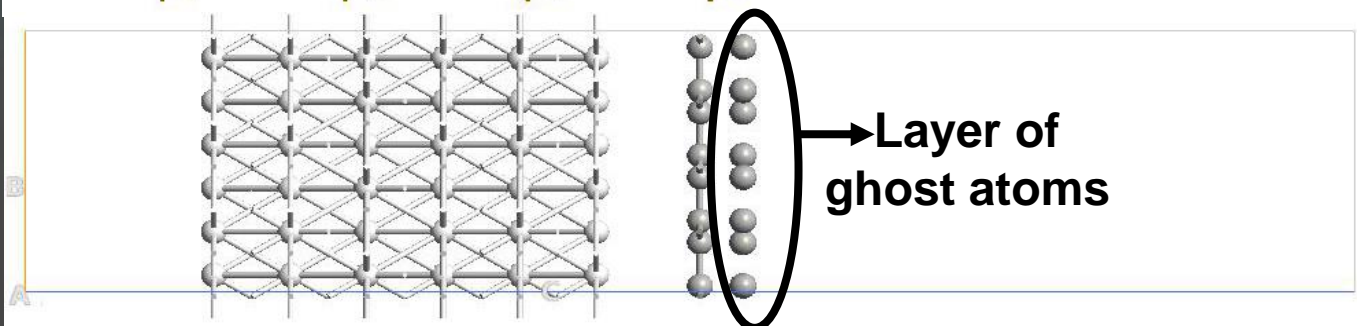
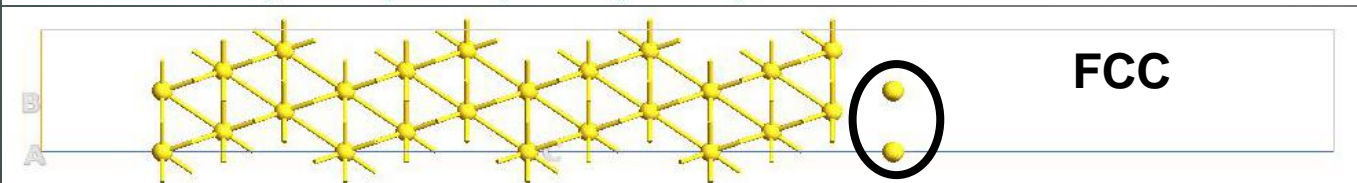
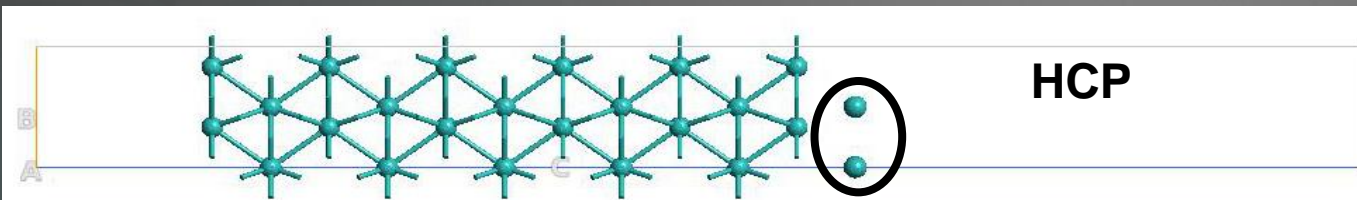
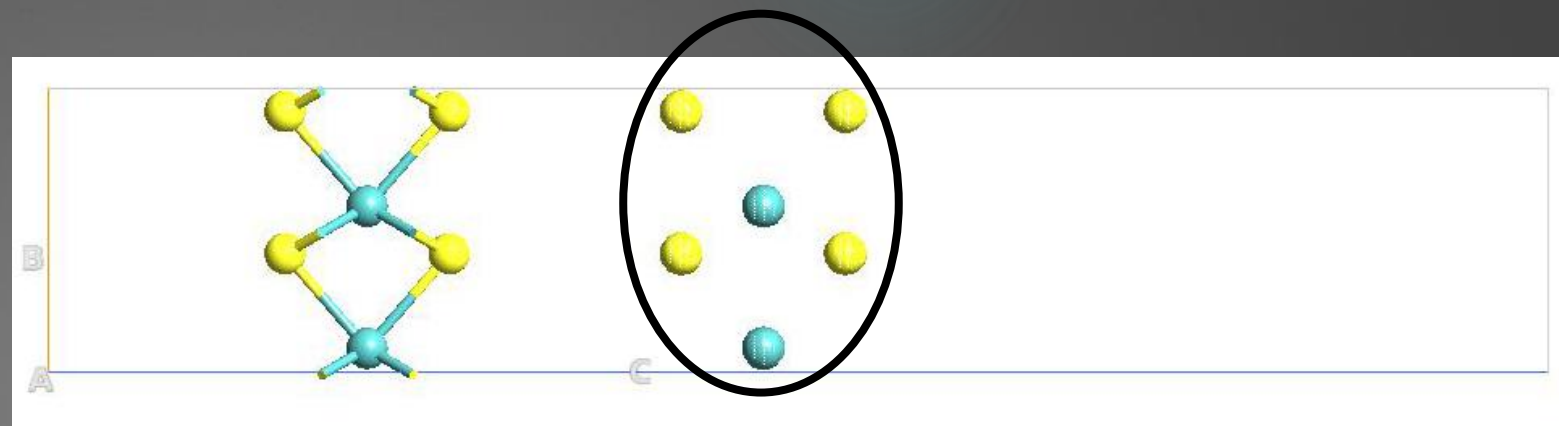
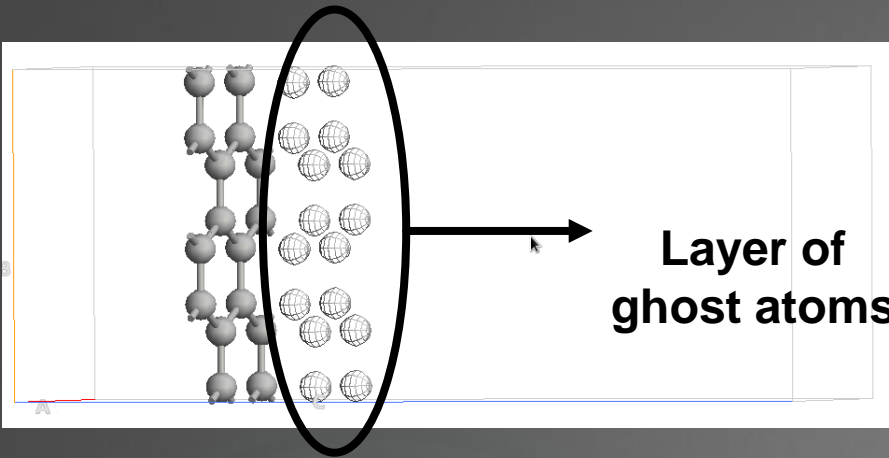


TABLE II: Area calculated between the interfacial sulfur atom of MoS₂ and carbon atom of graphene for various MoS₂-graphene-metal interface.

System	Area Under EDD between C and S atoms
MoS ₂ -G	1.7×10^{-7}
MoS ₂ -G-Au	-1.04×10^{-7}
MoS ₂ -G-Ag	3.42×10^{-7}
MoS ₂ -G-Ti	5.62×10^{-6}
MoS ₂ -G-Pt	-3×10^{-7}
MoS ₂ -G-Ru	8.1×10^{-6}

WORK FUNCTION CALCULATION

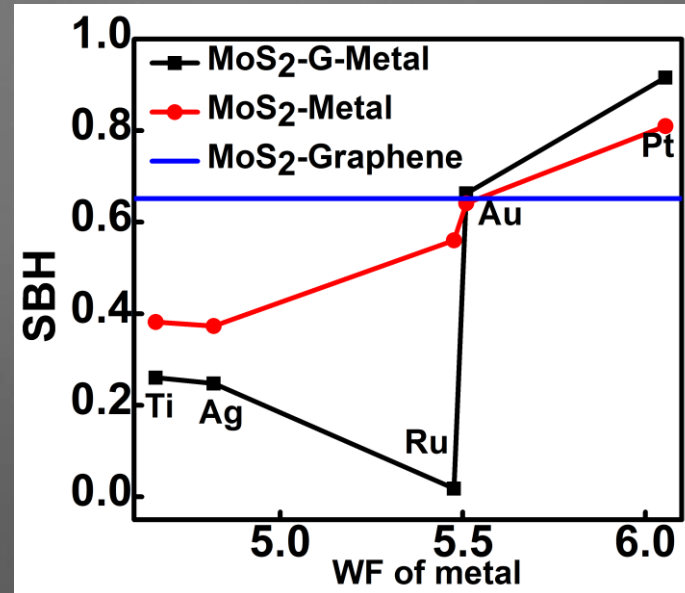
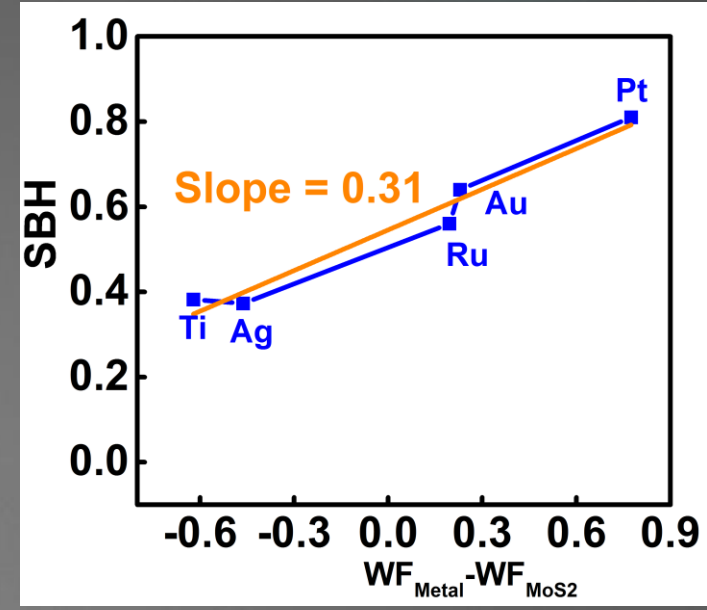
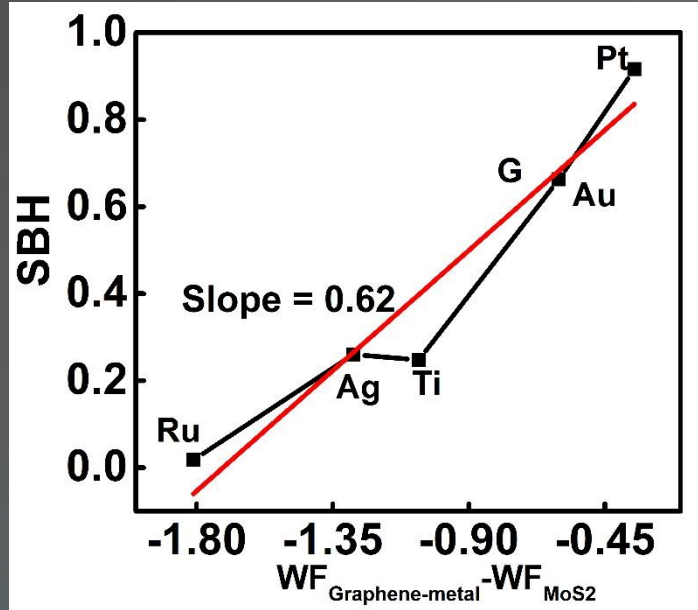


Metal	Calculated	Reported
Titanium	4.6589	4.56
Silver	4.81793	4.74
Ruthenium	5.47582	5.14
Gold	5.50947	5.54
Platinum	6.05502	6.13

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 MoS₂ 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 MoS₂-metal interface, the projected dispersion of MoS₂ remains preserved in any MoS₂-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 MoS₂-metal contact.
- ❖ These understandings would provide a direction in developing high performance transistors involving hetero atomic layers as contact electrodes.

QUESTIONS??