NANO-SCALE DEVICE RESEARCH LABORATORY

Practice Thinking.....

INVESTIGATIONS OF 2D MATERIAL METAL CONTACT USING DENSITY FUNCTIONAL THEORY

2D MATERIALS

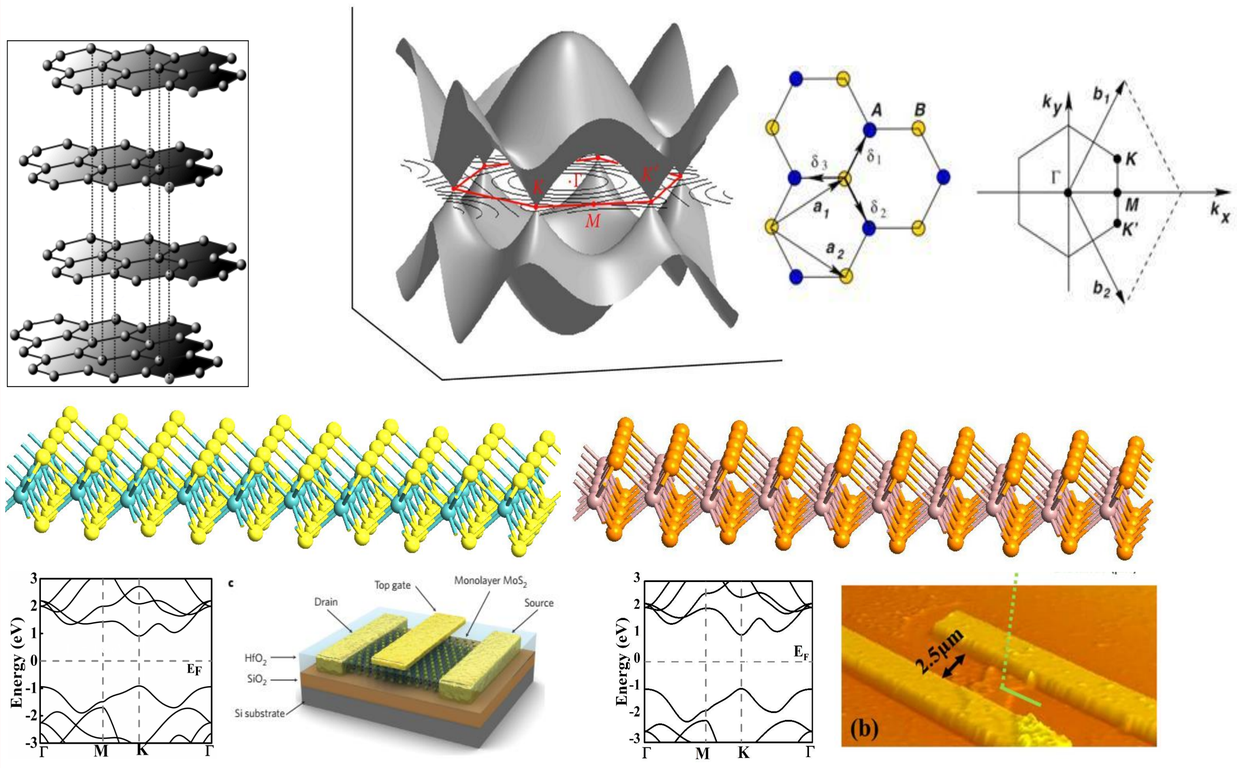
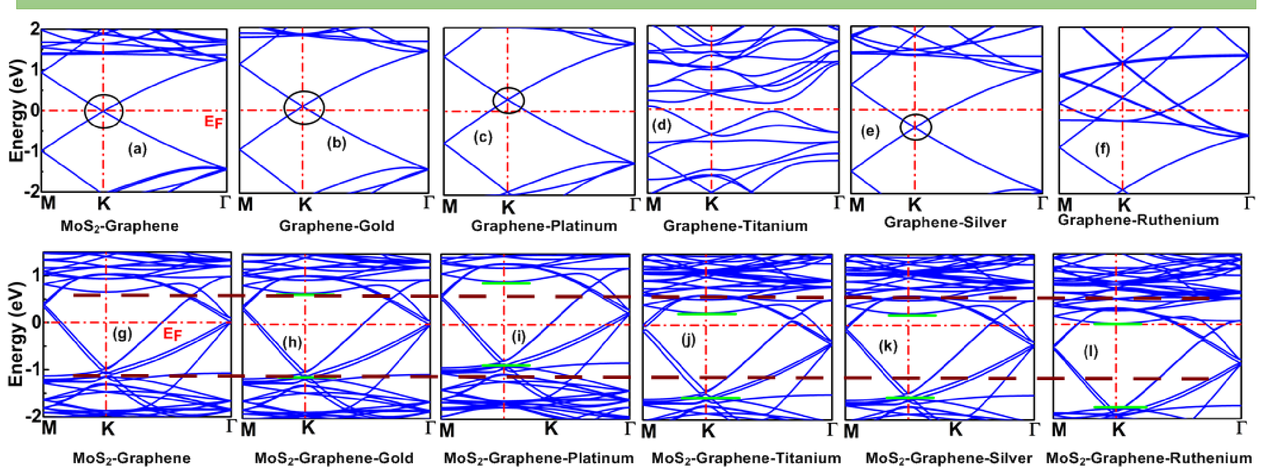


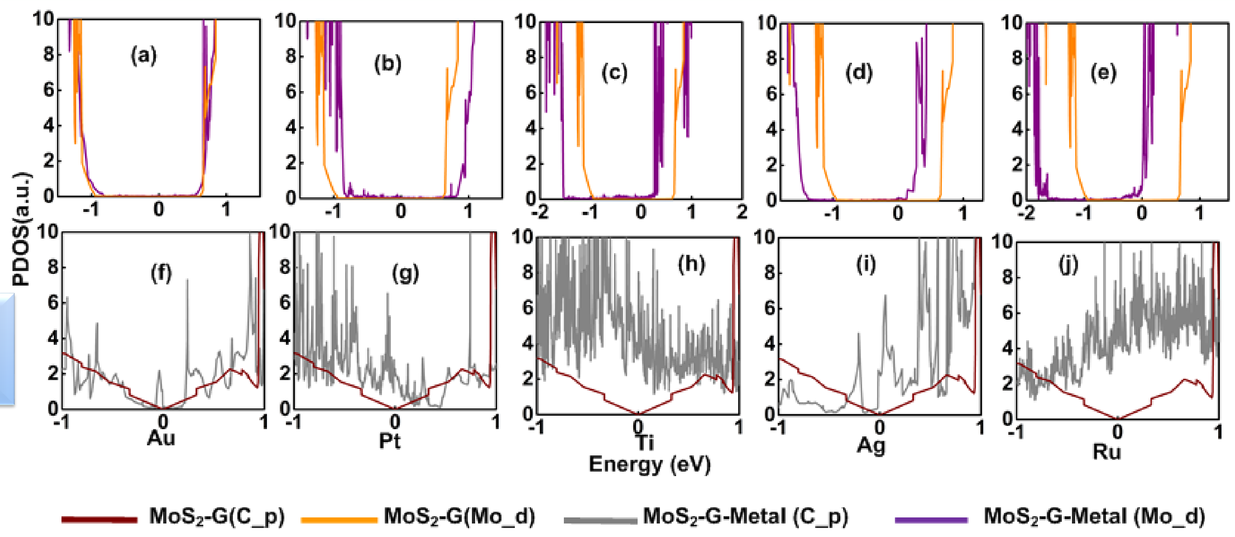
TABLE I: Strain applied in all the interfaces, Calculated equilibrium distances (z-direction) corresponding to minimum binding energy(BE), BE values, Dirac Cone shift only applicable to physisorped interfaces involving graphene, Schottky Barrier Heights(p-type and n-type) corresponding to interfaces with MoS_2, Band gap (Eg) values for MoS_2-metal interface and MoS_2-graphene-metal interface calculated by adding p-type SBH and n-type SBH

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
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

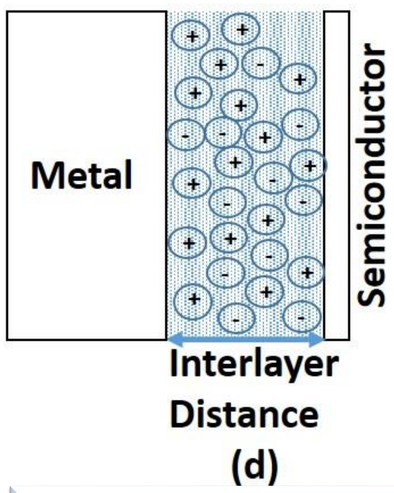
SBH EVALUATION



ORBITAL HYBRIDIZATION

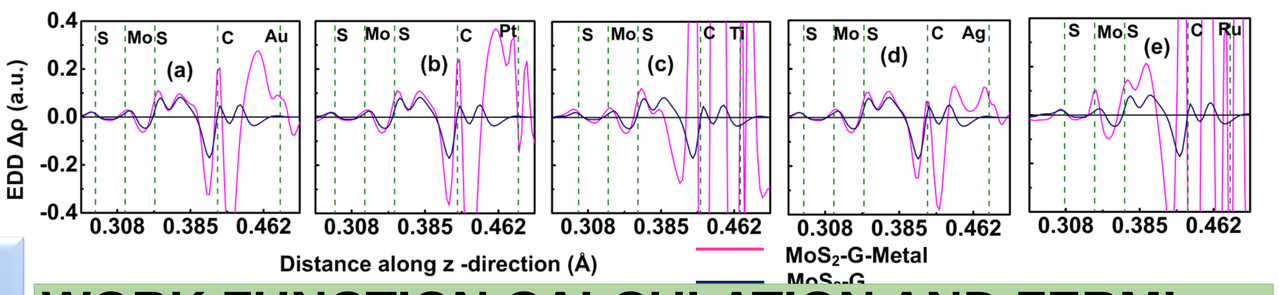


METAL SEMICONDUCTOR INTERFACE



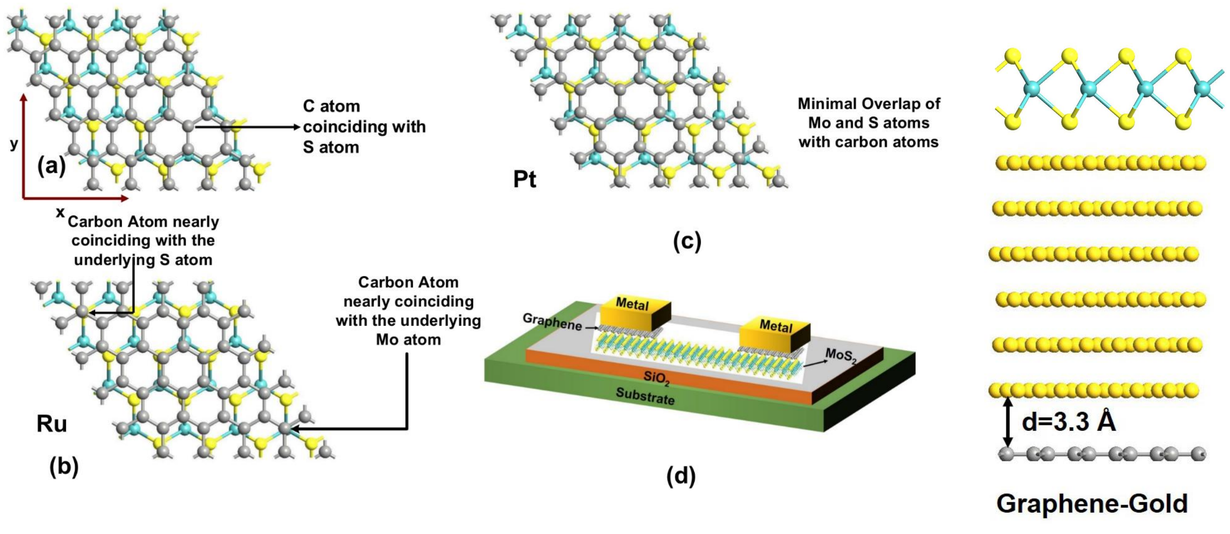
- The metal semiconductor depicts a Schottky or an Ohmic behavior. $\phi_{B,n} = \varphi_M - \chi_{SC}$
- Schottky Mott Rule $S_\phi = \frac{\partial \phi_{B,n}}{\partial \varphi_M}$
- Fermi-level Pinning
- Fails when the interfacial chemistry come into picture.
- More governed by the charge transfer at the interface.
- SBH is given by n-SBH = E_C-E_F , p-SBH = E_F-E_V

CHARGE DENSITY DIFFERENCE



SBH MODIFICATION USING GRAPHENE INSERTED MOS_2-METAL CONTACT

INTERFACE GEOMETRY



WORK FUNCTION CALCULATION AND FERMI LEVEL PINNING