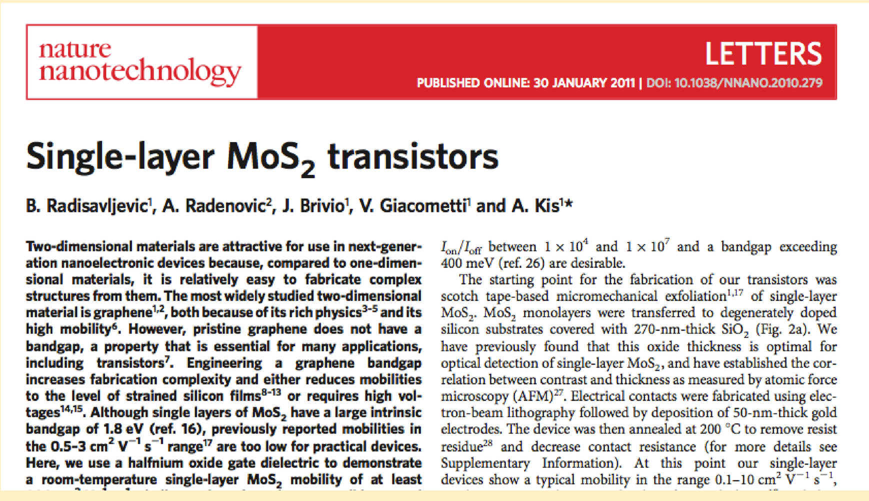
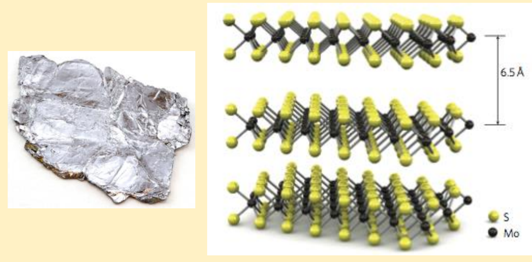
EECS Research Students Symposium – 2017

Atomistic Modeling of Phase-engineered MoS_2 Channel for the Decananometer Scale Digital Switches

Overview





- Abundance in nature and commonly used as lubricant

- Bandgap ~ 1.2 to 1.8 eV
- Thermal Conductivity(monolayer) @ RT ~ (34.5 ± 4) W/mK
- No dangling bonds
- Max. current density ~5×10⁷ A/Cm²
  50 times higher than Cu, But 5-10 times lower than graphene
- Stability up to 1100° C (in inert temp.)
- Effective mass
- Mobility

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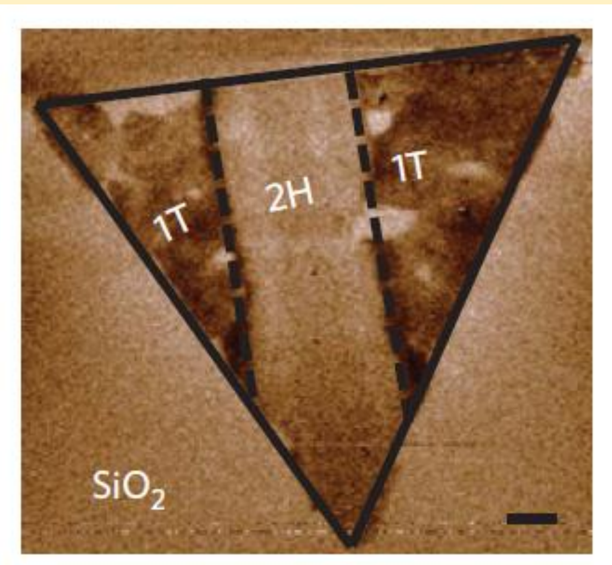
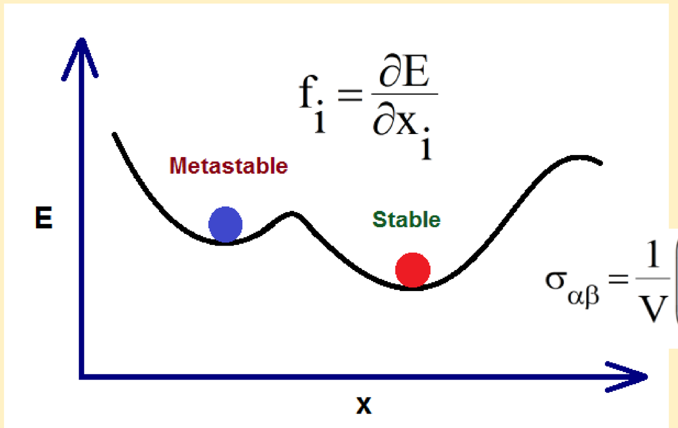
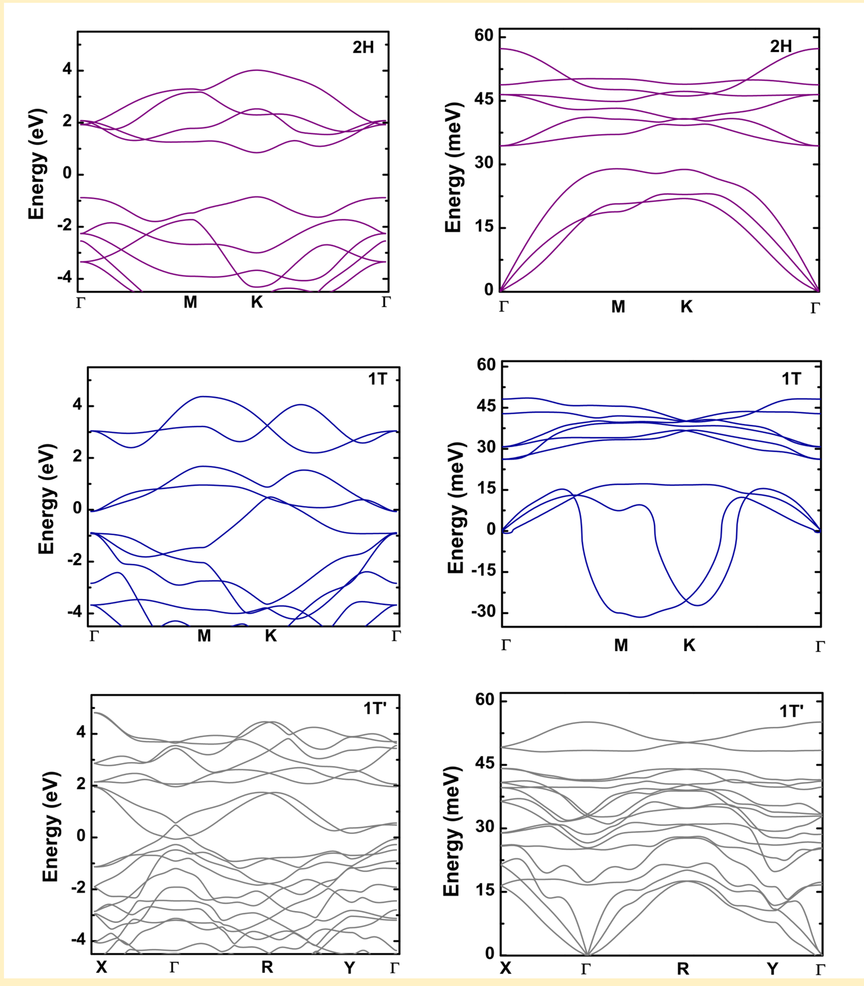
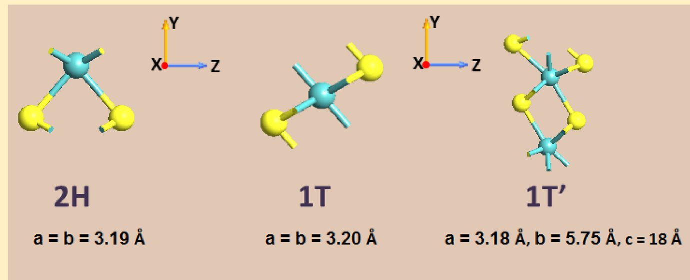




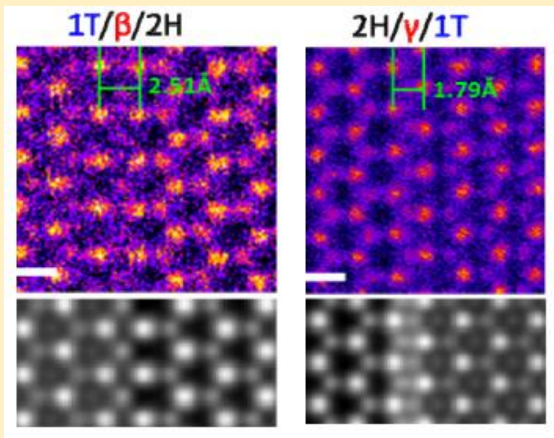
Ref :- Rajesh Kappera et al., NATURE MATERIALS, vol. 13, 2014

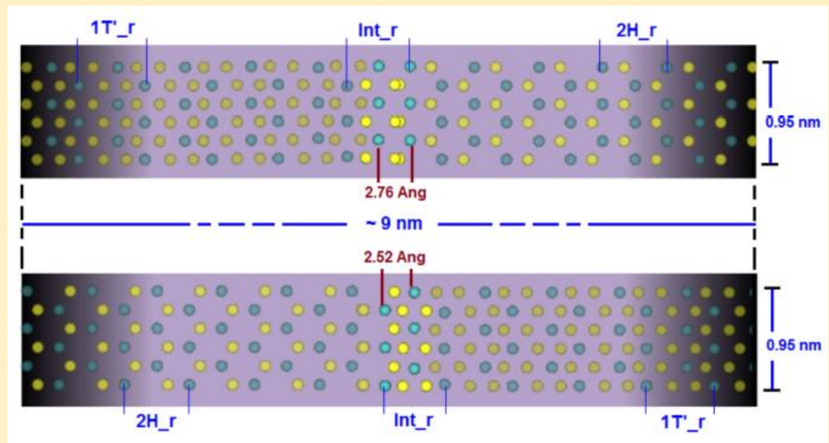
✓ Devices with 1T phase electrodes ~
Show much better performance compared the devices with 2H phase contacts





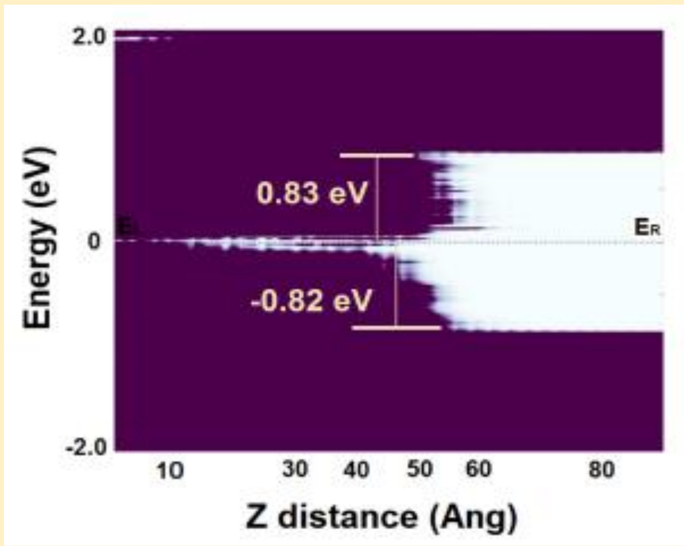
- The 'Mo'-'Mo' distance at the β phase boundary is calculated as 2.76 Ang
- Z-distance between 'Mo'-'Mo' atoms at the γ phase boundary is found to be 2.52 Ang

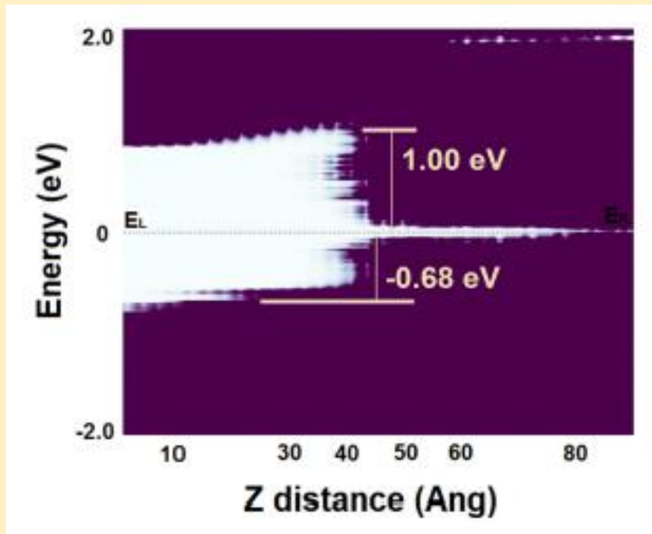




➢ Atomistic models of the in-plane hetero-phase structures with β and γ phase boundaries

Ref :- D. Saha, S. Mahapatra, Applied Physics Letters , 108, 253106, 2016
Ref :- Y-C. Lin, D. O. Dumcenco, Y-S. Huang, and K. Suenaga, *Nature Nanotechnology*, 9, 2014





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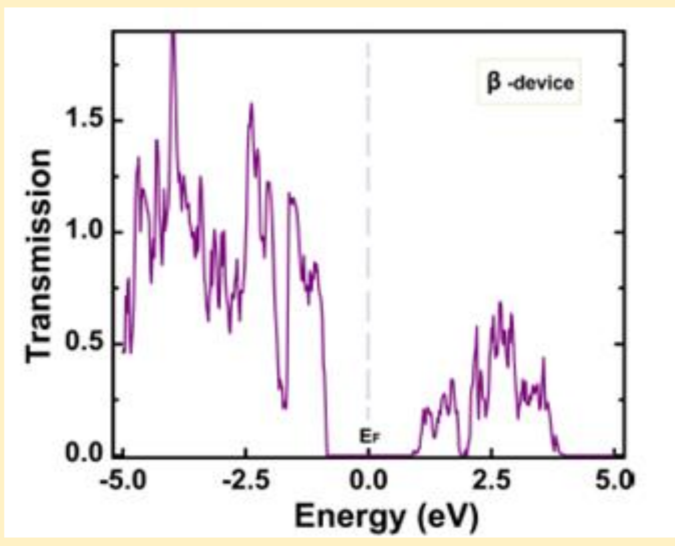
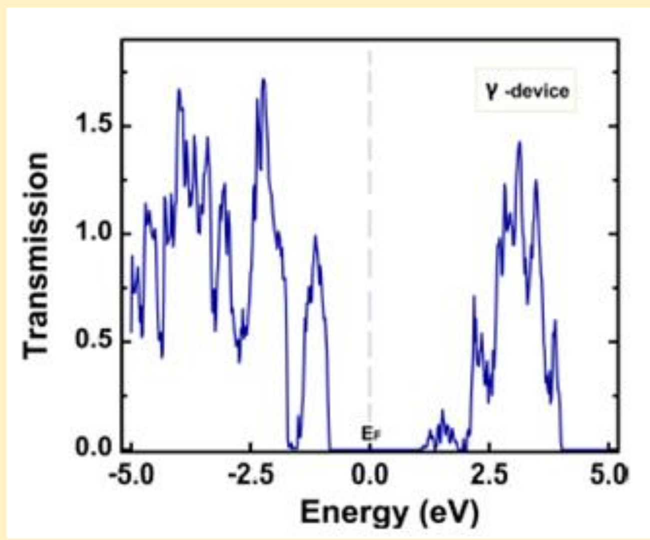
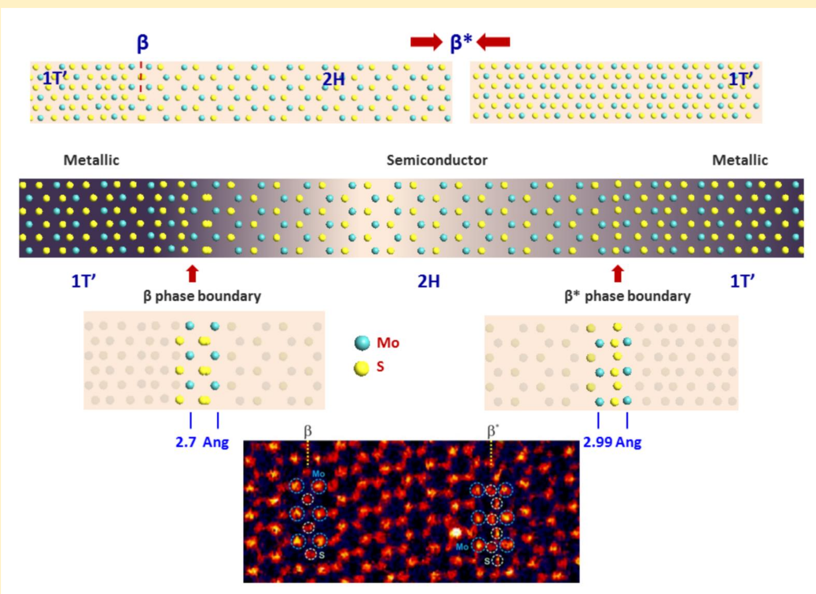


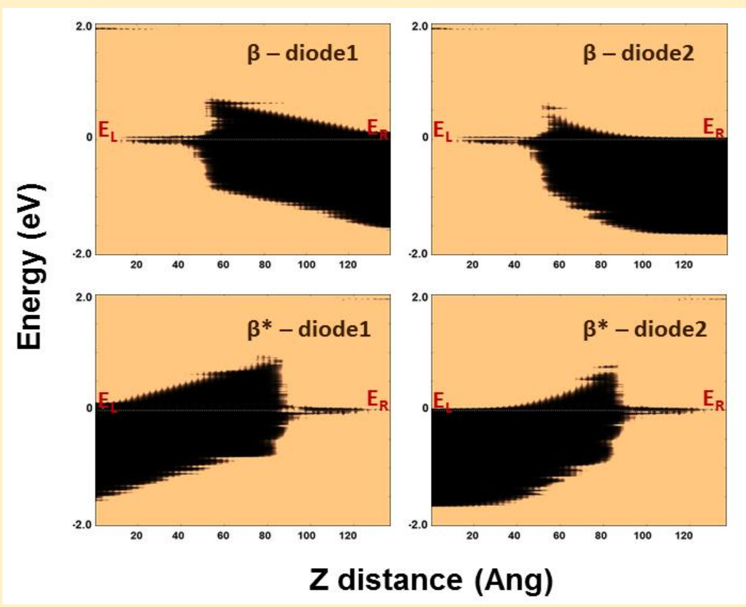


✓Up-spin components of transmission spectra (obtained at zero bias) of the β-device and the γ-device respectively

M-S-M heterophase MoS_2 structure

✓ Asymmetric Junctions in Metallic-Semiconducting-Metallic heterophase MoS_2~
atomic patterns at β and β* phase boundaries





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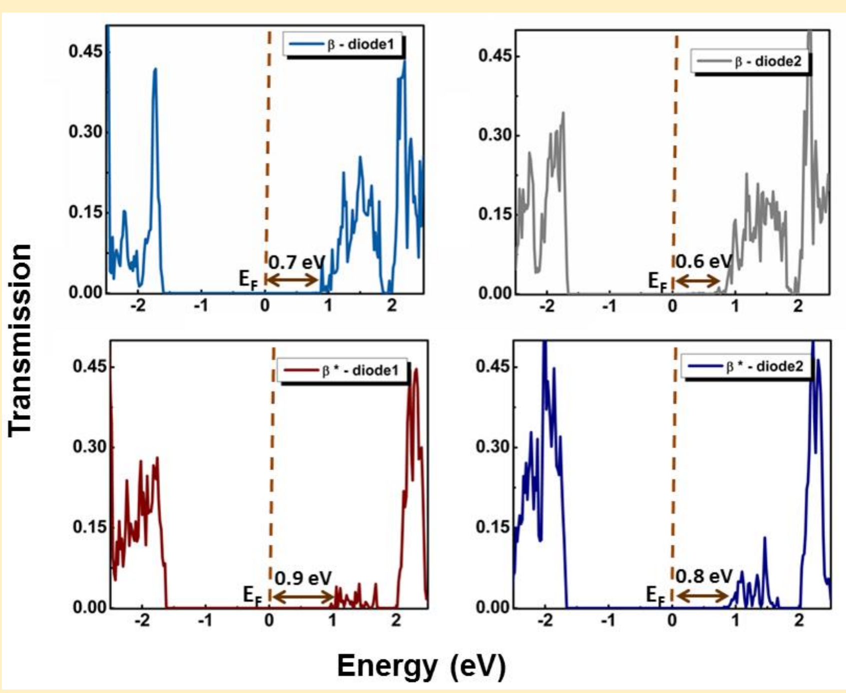

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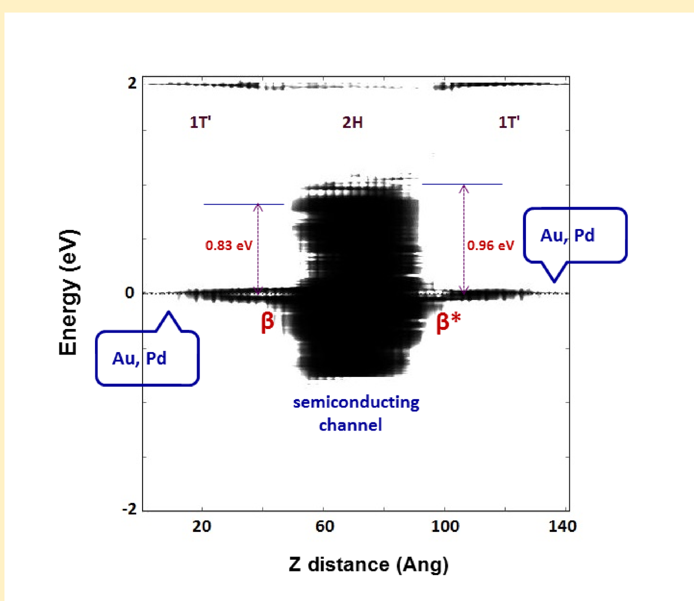
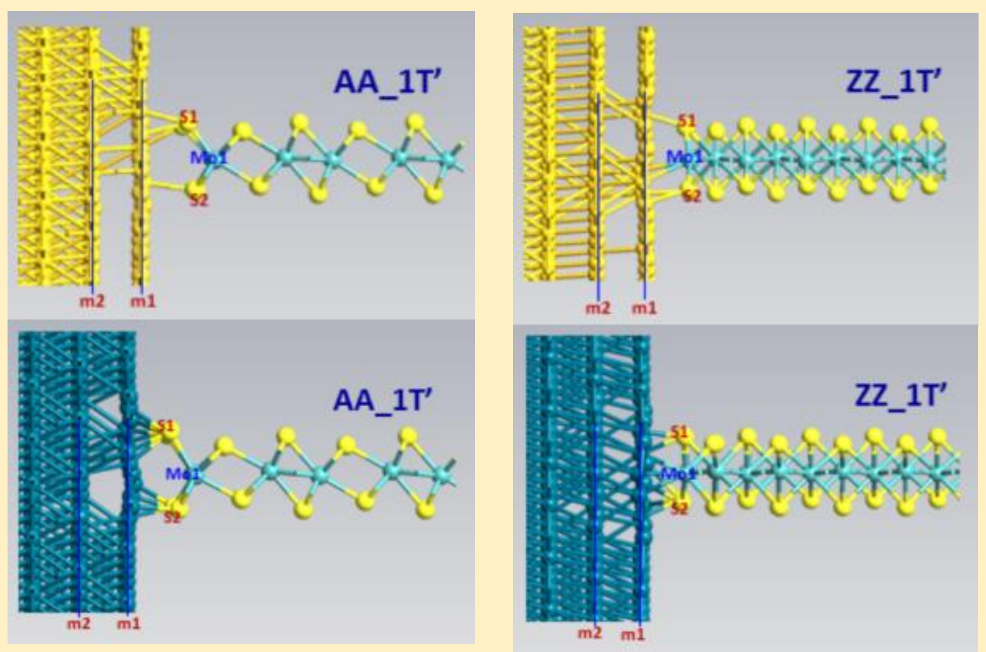


Energy-position resolved LDOS diagram for the hetero-phase MoS_2 structure. The metallic 1T' extensions can be used to achieve excellent impedance matching with the metal contacts (e.g., Au, Pd, etc.). For this plot, min. and max. values of device density of states (1/eV) are taken as 0 and 0.05 respectively.

Metal 1T' MoS_2 interfaces



Device structures	R (Ω.μm)
AA_1T'	55.9
Au_AA_1T'	293
Pd_AA_1T'	641
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Au_ZZ_1T'	37.08
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Ref :- D. Saha, S. Mahapatra, Physical Chemistry Chemical Physics, Royal Society of Chemistry

➢ Dipankar Saha* and Santanu Mahapatra^ [*dipsah_etc@yahoo.co.in, ^santanu@dese.iisc.ernet.in]
Nano-Scale Device Research Laboratory, Department of Electronic Systems Engineering, Indian Institute of Science Bangalore, Bangalore 560012, India

EECS Research Students Symposium – 2017

INDIAN INSTITUTE OF SCIENCE
भारतीय विज्ञान संस्थान

INDIAN INSTITUTE OF SCIENCE, BANGALORE

Atomistic Modeling of Phase-engineered MoS_2 Channel for the Decananometer Scale Digital Switches

Dipankar Saha

PhD Student

Under the Supervision of Prof. Santanu Mahapatra

Department of Electronic Systems Engineering,
Indian Institute of Science,
Bangalore-560012

Introduction

nature nanotechnology
LETTERS
PUBLISHED ONLINE: 30 JANUARY 2011 | DOI: 10.1038/NNANO.2010.279

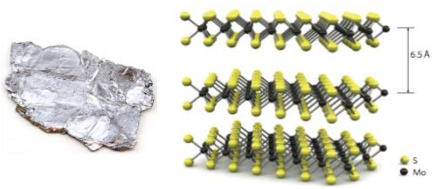
Single-layer MoS_2 transistors

B. Radisavljevic[1], A. Radenovic[2], J. Brivio[1], V. Giacometti[1] and A. Kis[1]*

Two-dimensional materials are attractive for use in next-generation nanoelectronic devices because, compared to one-dimensional materials, it is relatively easy to fabricate complex structures from them. The most widely studied two-dimensional material is graphene[1,2], both because of its rich physics[3-5] and its high mobility[6]. However, pristine graphene does not have a bandgap, a property that is essential for many applications, including transistors[7]. Engineering a graphene bandgap increases fabrication complexity and either reduces mobilities to the level of strained silicon films[8-13] or requires high voltages[14,15]. Although single layers of MoS_2 have a large intrinsic bandgap of 1.8 eV (ref. 16), previously reported mobilities in the 0.5–3 $cm^2 V^{-1} s^{-1}$ range[17] are too low for practical devices. Here, we use a halfnium oxide gate dielectric to demonstrate a room-temperature single-layer MoS_2 mobility of at least

I_{on}/I_{off} between 1×10^4 and 1×10^7 and a bandgap exceeding 400 meV (ref. 26) are desirable.

The starting point for the fabrication of our transistors was scotch tape-based micromechanical exfoliation[1,17] of single-layer MoS_2. MoS_2 monolayers were transferred to degenerately doped silicon substrates covered with 270-nm-thick SiO_2 (Fig. 2a). We have previously found that this oxide thickness is optimal for optical detection of single-layer MoS_2, and have established the correlation between contrast and thickness as measured by atomic force microscopy (AFM)[27]. Electrical contacts were fabricated using electron-beam lithography followed by deposition of 50-nm-thick gold electrodes. The device was then annealed at 200 °C to remove resist residue[28] and decrease contact resistance (for more details see Supplementary Information). At this point our single-layer devices show a typical mobility in the range 0.1–10 $cm^2 V^{-1} s^{-1}$,



- Abundance in nature and commonly used as lubricant

- Bandgap ~ 1.2 to 1.8 eV
- Thermal Conductivity(monolayer) @ RT ~ (34.5 ± 4) W/mK
- No dangling bonds
- Max. current density ~5×10^7 A/Cm^2

  50 times higher than Cu, But 5-10 times lower than graphene
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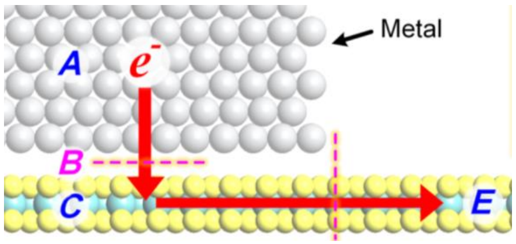
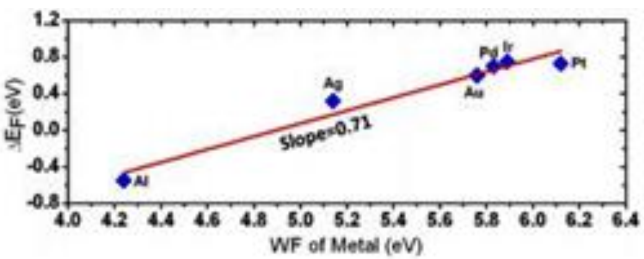
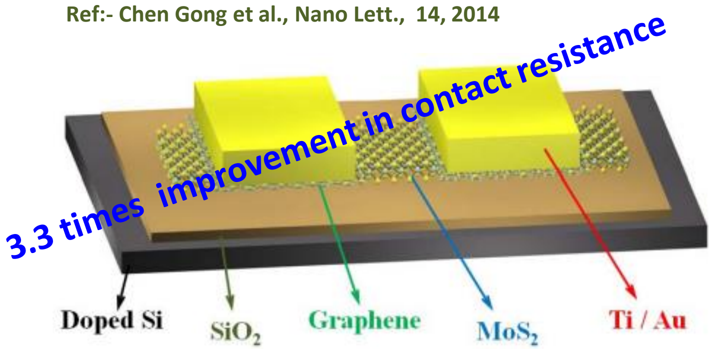
Introduction (cntd.)



Ref: - Jiahao Kang et al., PHYSICAL REVIEW X 4, 031005 (2014)



Ref:- Chen Gong et al., Nano Lett., 14, 2014



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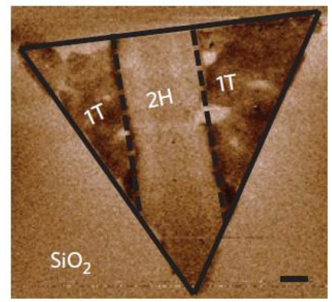
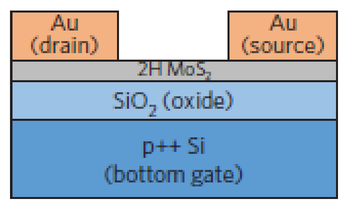
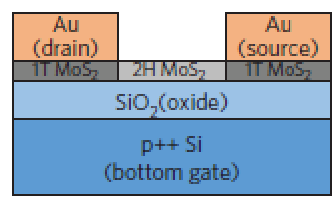
✓ **Devices with 1T phase electrodes→**

Show much better performance compared the devices with 2H phase contacts







Property	2H phase contacts	1T phase contacts
ON Current (μA /μm)	30	85
Transconductance (μS /μm)	1.4	3.8
Mobility (cm^2/V-s)	19	46
ON / OFF ratio	10^7	10^8

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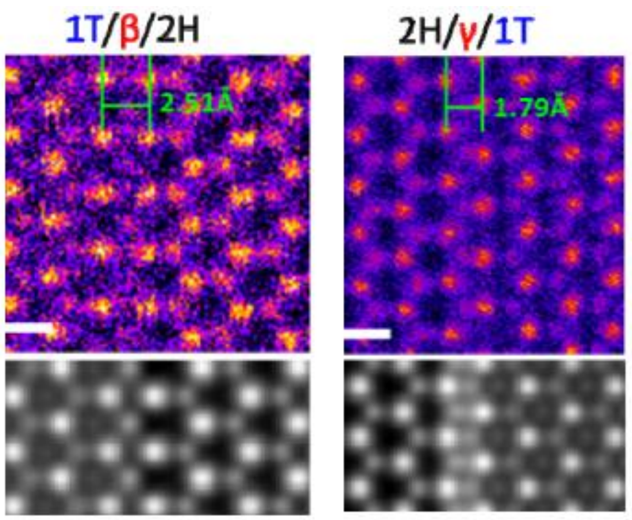
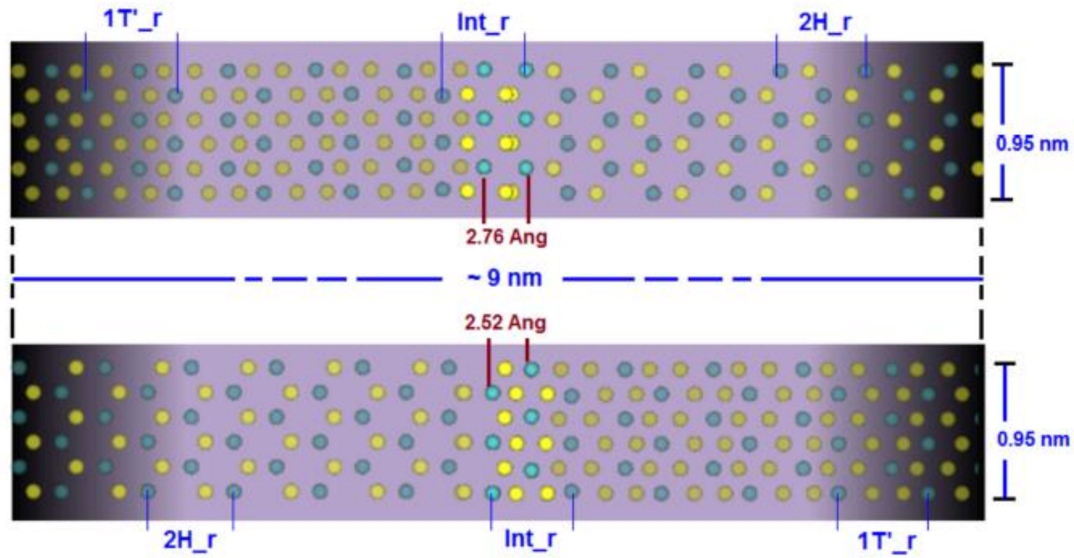
Metallic to Semiconducting Phase Boundaries





✓ **Atomistic models of the in-plane hetero-phase structures with β and γ phase boundaries**

- **The ‘Mo’-‘Mo’ distance at the β phase boundary is calculated as 2.76 Ang**
- **Z-distance between ‘Mo’-‘Mo’ atoms at the γ phase boundary is found to be 2.52 Ang**

Perhaps, the slight differences in the ‘Mo’-‘Mo’ distances at the boundaries, may have originated from the choice of our unit cells, lattice constants

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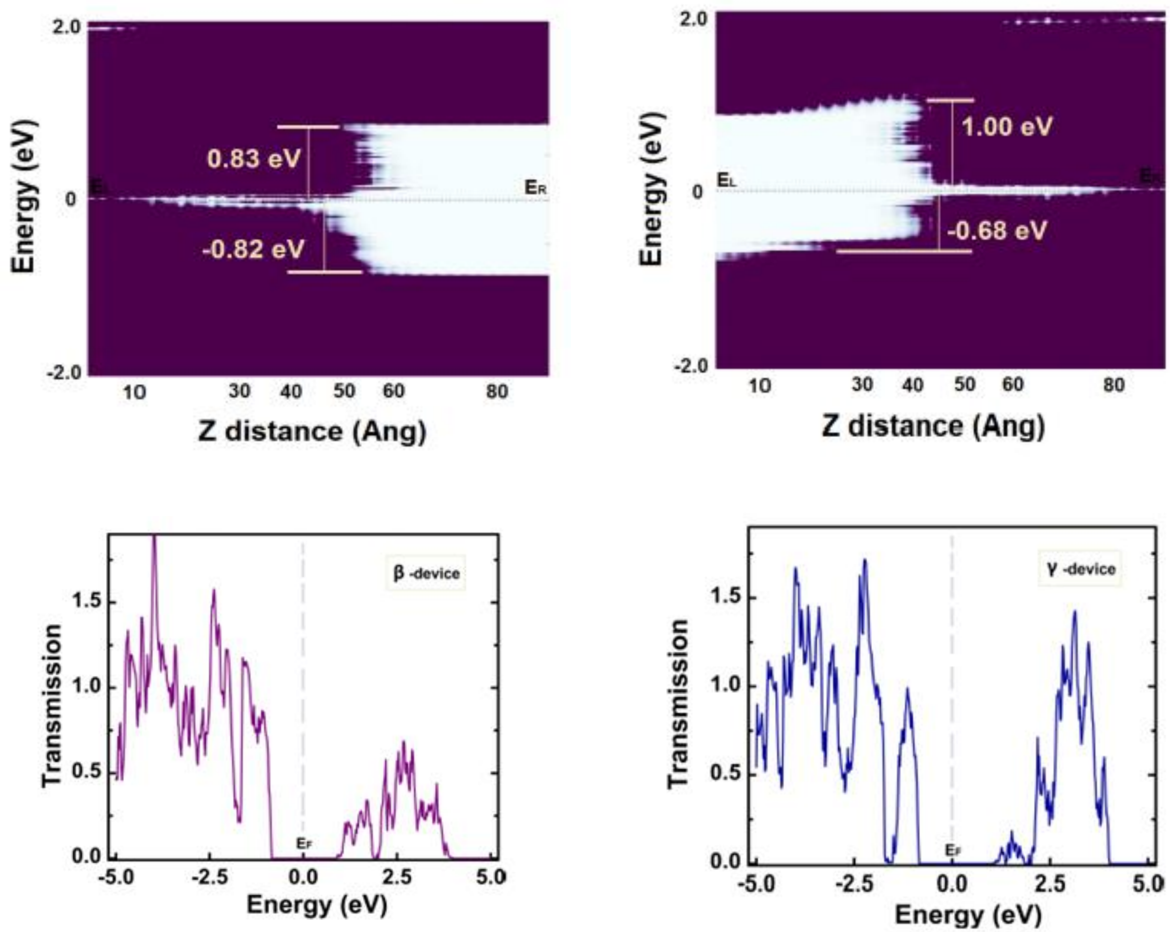

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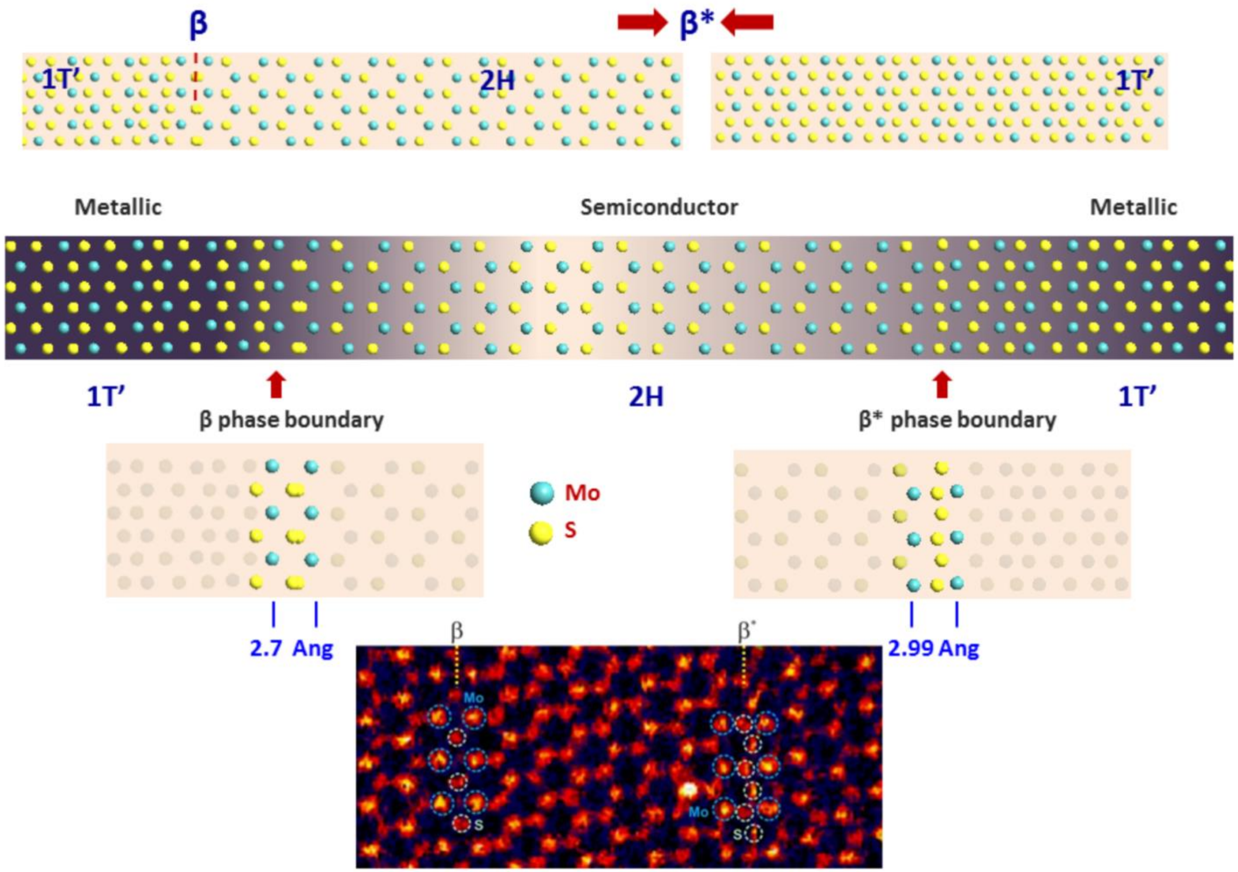

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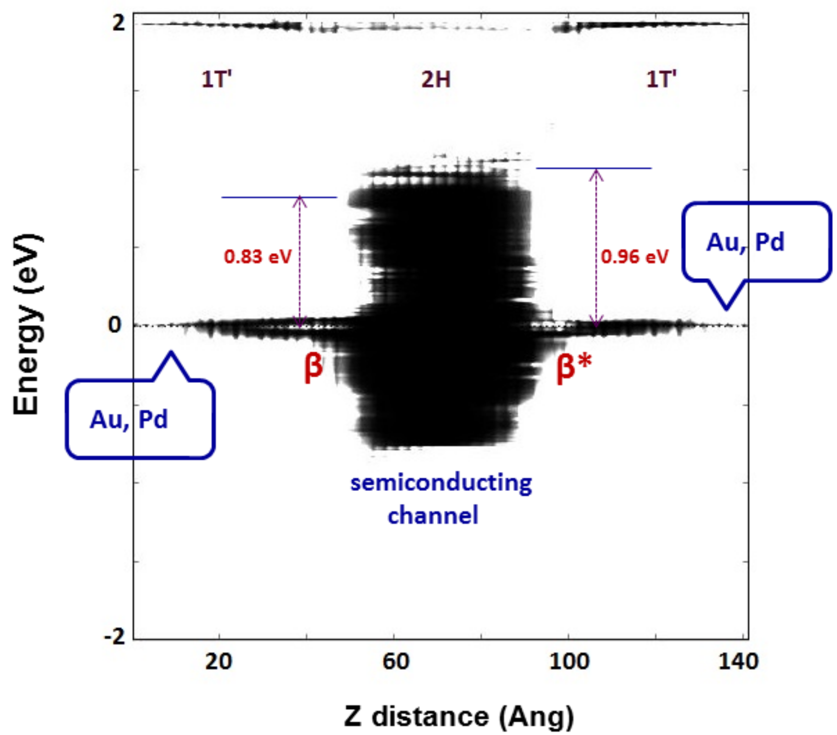

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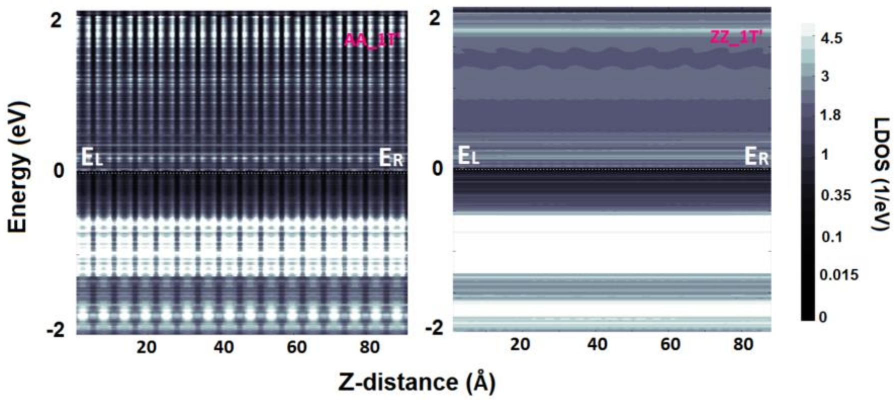
1T’ monolayer MoS_2 and its metal interfaces



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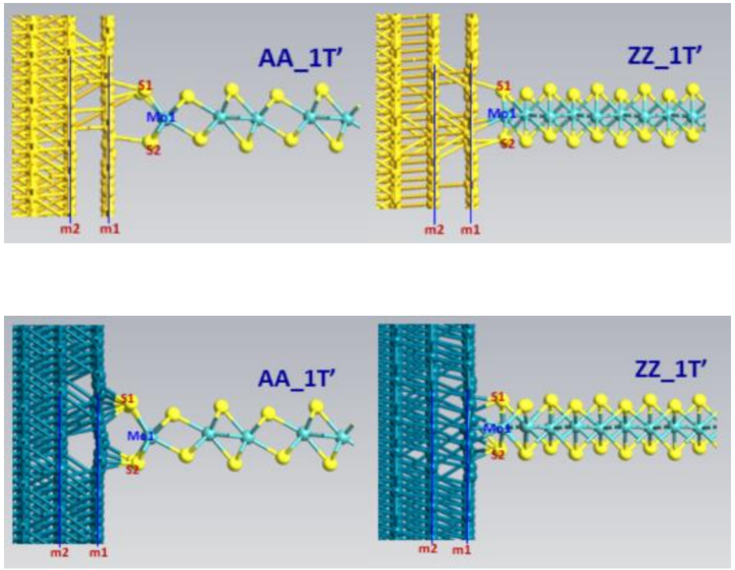

Ref :- D. Saha, S. Mahapatra, Physical Chemistry Chemical Physics, (Under Review)

Summary

- ✓ **We have designed Atomistic Model of the planar hetero-phase structures of monolayer MoS_2, having two disparate phase transition regions**
- ✓ **We explored Asymmetric Junctions in M-S-M hetero-phase structure, and obtained the charge carrier transport through the β and β* phase boundaries**
- ✓ **We have also investigated the orientation dependent charge carrier transport in the metal (Au and Pd) interfaces of 1T′ MoS_2**

- **The key advantage of such devices is their 1T′ extension region which can effectively be contacted with various metals for significantly reducing the Schottky-limited transport**

Thank You