Defect Assisted Metal-TMDs Interface Engineering: A First Principle Insight

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Introduction: 2D materials make the scientific land more fertile to harvest future generation of high-performance electronic devices. Among these, TMDs are more promising for switching applications due to its band gap and stability over Graphene and Phosphorene respectively. Despite of these properties, performance of the TMDs FET is not achieved to its expectation yet due to high contact resistance at the metal-TMDs interfaces. Different metal-TMDs interfaces have been explored for contact resistance reduction [1], [2], [3] but, a systematic study of metal induced gap states [MIGS] for TMDs and corresponding engineering to improve the contact resistance is missing yet. To explore the gap, we have done systematic study of interaction of different metals (*Au, Cr, Ni* and *Pd*) with MoS_2, $MoSe_2$, WS_2 and WSe_2 followed by impact of chalcogen vacancy on corresponding interactions using Density Functional Theory (DFT). Chalcogen vacancy reduces all the metal-TMDs bond distance which can reduce corresponding contact resistance due to reduction in the tunneling barrier width. Defect engineering also converts intrinsic n-type Pd-TMDs contacts into p-type which can help in MoS_2 based CMOS circuit in future.

Computational details: QuantumATK package [4] was used for DFT computations. A 5x5 super cell of monolayer TMDs (mTMDs) were taken (Fig. 1) and ~15 Å vacuum space was added on both sides of the plane. *Au, Cr, Ni* and *Pd* metals were selected for analysis which covers low and high work functions as well as electronegativities. Four atoms of corresponding metal were kept above the chalcogen atoms of the TMDs to capture more insights of interface chemistry. Periodic boundary condition was applied to replicate bulk mTMDs planes. All the simulating modules were optimized with 0.01 eV/Å and 0.001 eV/Å^3 force and energy cutoffs respectively. Perdew-Burke-Ernzerhof (PBE) form of generalized gradient approximation (GGA) functional was used with 5x5x1 k point sampling. Grimme DFT-D2 Van der Walls (vdW) correction was considered to capture long range metal TMDs vdW interactions.

Results and discussion: Schottky barrier height (SBH) and tunnel barrier width (vdW gap) are carrier transport killers at the metal-TMDs interface (Fig. 2) while Metal Induced Gap States (MIGS) can kill or enhance carrier transport depends on Fermi level pinning position determined by trap state position and its density of states. Here, we discuss metal selection based on MIGS and fermi level position (to determine SBH) and chalcogen vacancy (defect) engineering which can help in understanding of metal-TMDs interfaces and reduction of contact resistance.

Ni has good bonding affinity with MoS_2, $MoSe_2$, and WS_2 among the metals while Pd has good affinity with WSe_2 (Fig. 3). Due to contact resistance dependency on the vdW gap, Ni can give least contact resistance with MoS_2, $MoSe_2$, and WS_2 while Pd with WSe_2. SBH at the contact depends on the metal work function and fermi level pinning position due to MIGS. Among computed results (Fig. 4 to Fig. 8), Au (0.32 eV) can have least Schottky barrier height (~ (E_c-E_F)) with MoS_2 (Fig. 5), Cr (0.17 eV) and Ni (0.19 eV) with $MoSe_2$ (Fig. 6), Cr (0.26 eV) with WS_2 (Fig. 7) and, Ni (0.12 eV) with WSe_2 (Fig. 8). Based on the tunnel and Scottky barriers analysis, Ni can give least contact resistance among the other metals for $MoSe_2$ and WSe_2, Ni or Au (or alloy of both) can be good for MoS_2 and, Ni or Cr (or alloy of both) can be good for WS_2.

Creating chalcogen vacancy at the interface reduces vdW and the method is consistent for all the TMDs-metal combinations (Fig. 9). Intrinsic metal-TMD interface has vdW gap due to unavailability of bonding orbitals in the chalcogen. Once chalcogen (S, Se) vacancy is created, corresponding bonded transition metal of the TMDs (Mo, W) has unbounded orbitals which overlaps with contact metal hence enhances the metal-TMDs bonding which can reduce contact resistance due to tunnel barrier (vdW) reduction. Defect engineering also gives clue of TMDs-Pd based p-type devices. Intrinsic TMDs-Pd interfaces are n-type (Fig. 5 to Fig. 8). When chalcogen vacancy is created, corresponding interface becomes p-type behavior as show in Fig. 10. The behavior is consistent with all the TMDs-Pd interfaces.

Conclusion: Studied TMDs-metal interfaces has revealed that chalcogen vacancy engineering is a promising method for TMDs-metal contact resistance reduction. It can also be used for n-type to p-type conversion of TMDs-Pd based devices. We have also explored that Ni can be the optimum contact metal for $MoSe_2$ and WSe_2 while Ni or Au (or alloy of both) and Ni or Cr (or alloy of both) can be optimum option for MoS_2 and WS_2 respectively.

References: [1] Igor Popov, et. al.,PRL 108, 156802 (2012). [2] Jiahao Kang, et. al., IEDM 12. [3] Le Huang, et. al., PRB 96, 205303 (2017). [4] QuantumATK, version 2017.2, Quantumwise, Copenhagen, Denmark.

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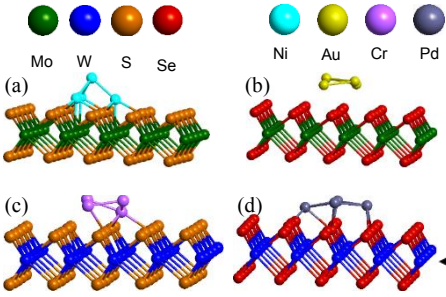

Fig. 1. Optimized intrinsic interface modules of (a) MoS_2-Ni, (b) $MoSe_2$-Au, (c) WS_2-Cr and (d) WSe_2-Pd. Similar modules have been simulated for all other combinations (Fig 3).

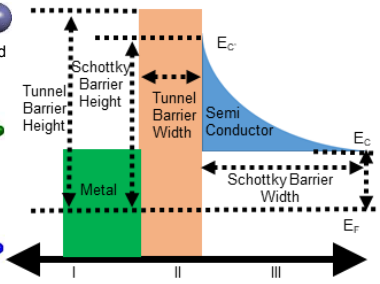

Fig. 2. Schematic of the carrier transport barriers at the metal-TMDs interfaces. Tunnel barrier width is equivalent to metal-TMDs bond (interfacial) distances while Schottky barrier is difference between CBM and Fermi level (E_C-E_F).

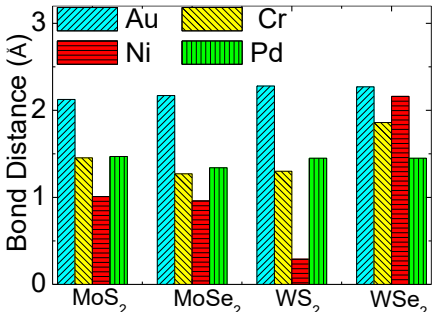

Fig. 3. Optimized bond (interfacial) distances of MoS_2, $MoSe_2$, WS_2 and WSe_2 with Au, Cr, Ni, and Pd. Au has maximum value among all the other metals across all the TMDs while Ni has least value with MoS_2, $MoSe_2$ and WS_2, and Pd has least value for WSe_2.

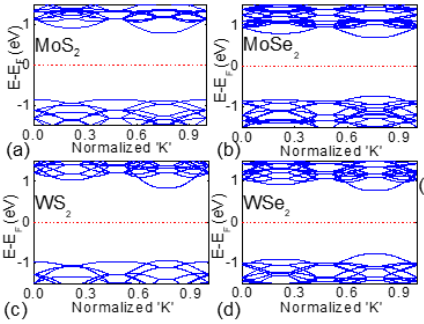

Fig. 4. Band structure of Intrinsic TMDs along: G→M→L→A→G→K→H→A. Similar band structure calculations have been done for MoS_2, $MoSe_2$, WS_2, and WSe_2 with Au, Cr, Ni and Pd (Fig. 5 to Fig. 8).

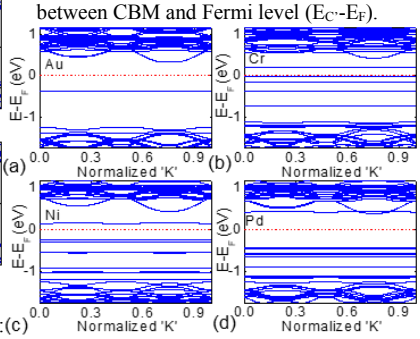

Fig. 5. Band structure of MoS_2 with metals. Au shows most n-type behavior with E_c-E_F = 0.32 eV followed by Pd (0.38 eV), Cr (0.42 eV) and Ni (0.43 eV). Cr and Ni have significant MIGSs near fermi level and VBM, Pd has significant MIGSs near VMB and one almost with CBM while Au has one in the mid gap.

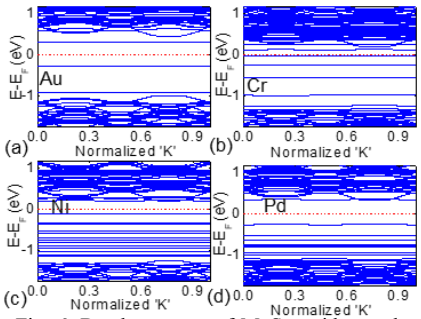

Fig. 6. Band structure of $MoSe_2$ with metals. Cr shows most n-type behavior with E_c-E_F = 0.17 eV followed by Ni (0.19 eV), Pd (0.31 eV) and Au (0.44 eV). Cr and Ni have significant MIGSs near CBM and VBM, Pd has significant MIGSs near VMB and one almost with CBM while Au has one MIGS in the mid gap and near CBM and VBM each.

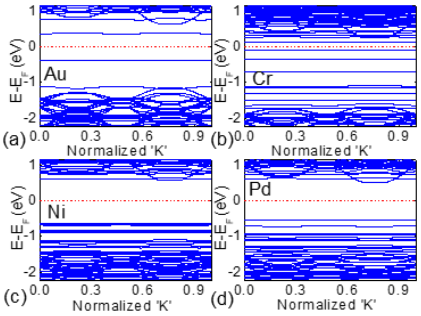

Fig. 7. Band structure of WS_2 with metals. Cr shows most n-type behavior with E_c-E_F = 0.26 eV followed by Pd (0.50 eV), Ni (0.62 eV) and Au (0.63 eV). Cr has MIGSs near CBM and VBM, Pd and Ni have significant MIGSs near VMB. Au has one each in the mid gap and near CBM.

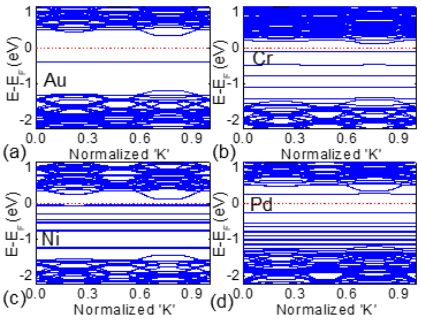

Fig. 8. Band structure of WSe_2 with metals. Ni shows most n-type behavior with E_c-E_F = 0.12 eV followed by Cr (0.24 eV), Pd (0.33 eV) and Au (0.33 eV). Cr has MIGSs near CBM and VBM, Pd has significant MIGSs near VMB, and Ni has most of the states in mid gap. Au has one MIGS each in the mid gap, near VBM and CBM.

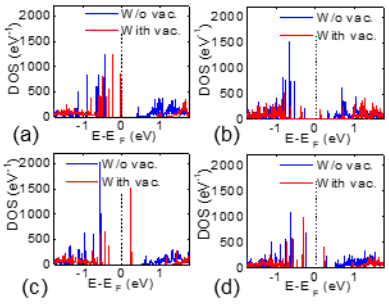

Fig. 10. Density of State (DOS) plot of (a) MoS_2-Pd, (b) $MoSe_2$-Pd, (c) WS_2-Pd and WSe_2-Pd, interfaces with and without vacancy engineering (Chalcogen vacancy). Fermi level is moved from near CBM to near VBM due to vacancy engineering in all the interfaces which reflects that vacancy engineering can be an effective technique for n-type to p-type conversion at the TMDs-Pd interfaces.

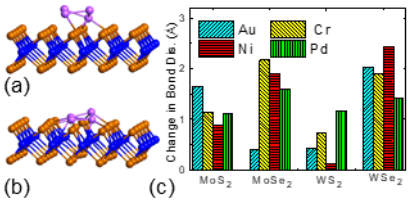

Fig. 9. Reduction in chalcogen-metal bond distance (ΔL) due to chalcogen Vacancy at the Optimized TMDs-metal interfaces. Reduction due to S vacancy in optimized WS_2-Cr from (a) Intrinsic to (b) one S vacancy at the central S position. Cr atoms come closer to the WS_2 due to S vacancy. (c) similar reduction in all other systems. Au, Cr, Pd and Ni has most reduction (ΔL) among other metals for MoS_2, $MoSe_2$, WS_2 and WSe_2 respectively. ΔL is bond distance of: optimized intrinsic module (L_{int}) – optimized module with Chalcogen vacancy (L_{vac}). ΔL is directly related to tunnel barrier reduction for carrier transport at the interfaces. Hence, Chalcogen vacancy engineering can be an effective technique of contact resistance reduction at the metal-TMDs interfaces.

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