Supplementary Information

Theoretical investigation of the vertical dielectric screening on defects for few-layered van der Waals materials

Amit Singh[a,b], Seunghan Lee[a], Hyeonhu Bae[a], Jahyun Koo[a], Li Yang[c] and Hoonkyung Lee[a,]*

[a]Department of Physics, Konkuk University, Seoul 05029, Korea

[b]Department of Mechanical Engineering, National Chiao Tung University, Hsinchu, 300, Taiwan, R.O.C.

[c]Department of Physics, Washington University in St. Louis, St. Louis, Missouri 63136, USA

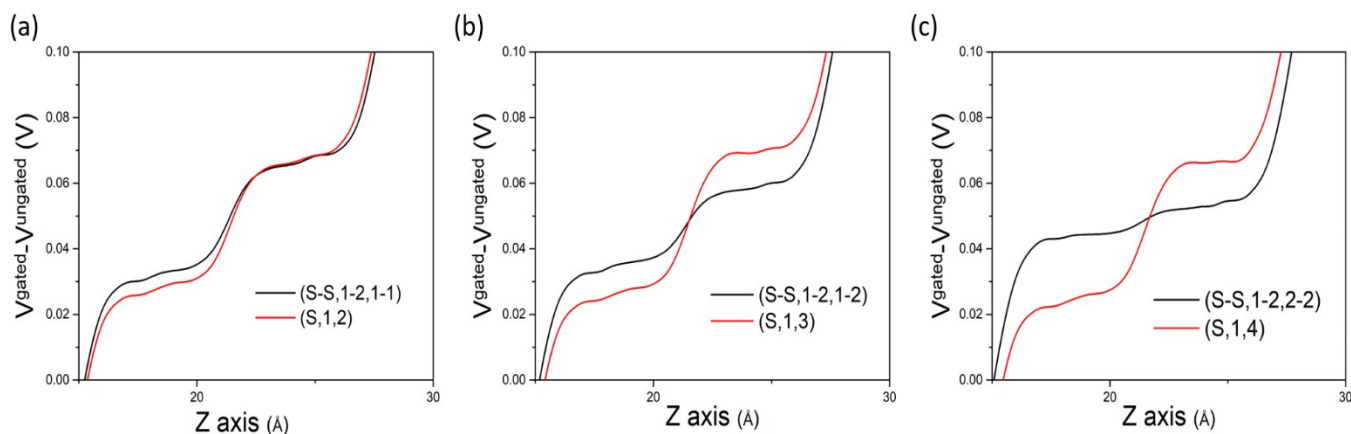The comparison between the distributed and non-distributed Sulphur vacancy:

Figure S1: The comparison of change in potential with and without gate field with S vacancy (Interlayer Distance 6.16 Å) (a) (S-S,1-2,1-1) and (S,1,2), (b) (S-S,1-2,1-2) and (S,1,3) and (c) (S-S,1-2,2-2) and (S,1,4).

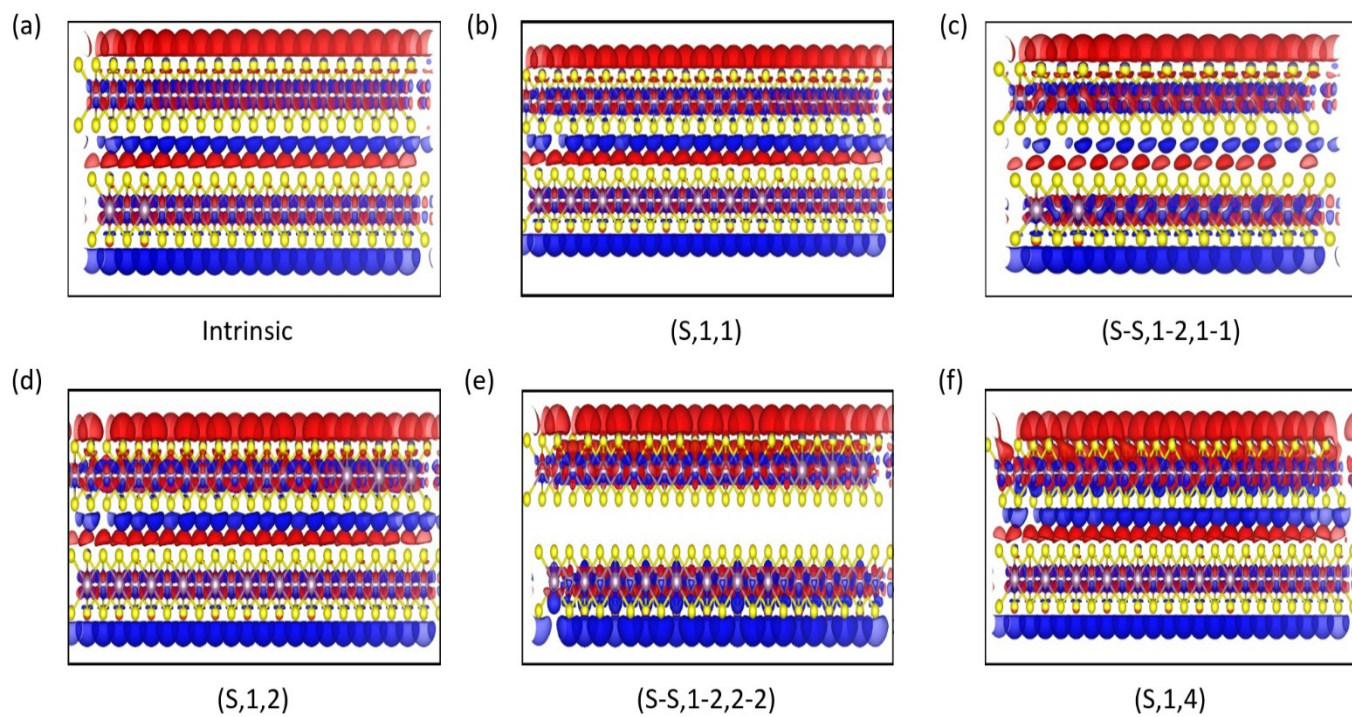The difference in charge density projected along Z-axis:

Figure S2: The difference in charge density with and without gate electric field (Interlayer Distance 6.16 Å) (a) Intrinsic, S vacancy cases (b) (S,1,1), (c) (S-S,1-2,1-1), (d) (S,1,2), (e) (S-S,1-2,2-2) and (f) (S,1,4).

The comparison between the distributed and non-distributed Molybdenum vacancy and the difference in charge density projected along Z-axis:
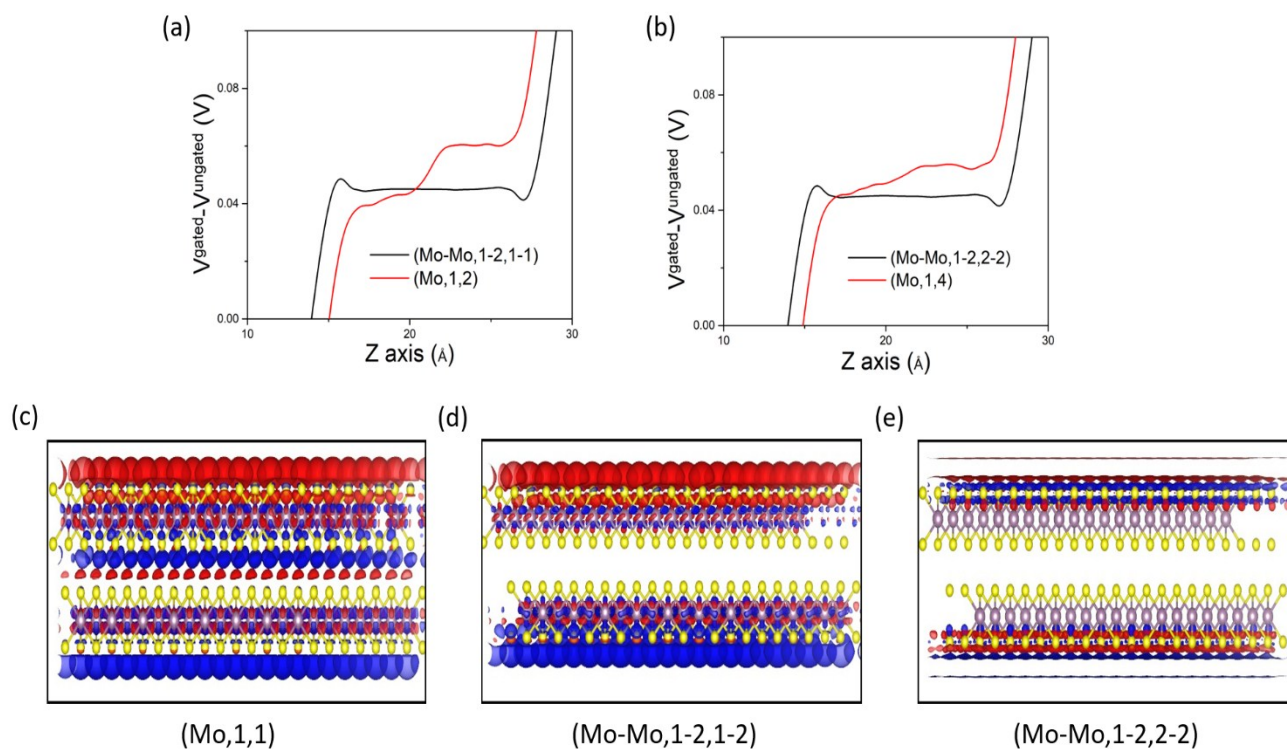

Figure S3: The comparison of change in potential with and without gate field with Mo vacancy (Interlayer Distance 6.16 Å) (a) (Mo-Mo,1-2,1-1) and (Mo,1,2), (b) (Mo-Mo,1-2,2-2) and (Mo,1,4) and the difference in charge density with and without gate electric field with Mo vacancy (c) (Mo,1,1), (d) (Mo-Mo,1-2,1-2) (e) (Mo-Mo,1-2,2-2).

The change in potential with and without gate field with different interlayer distance:
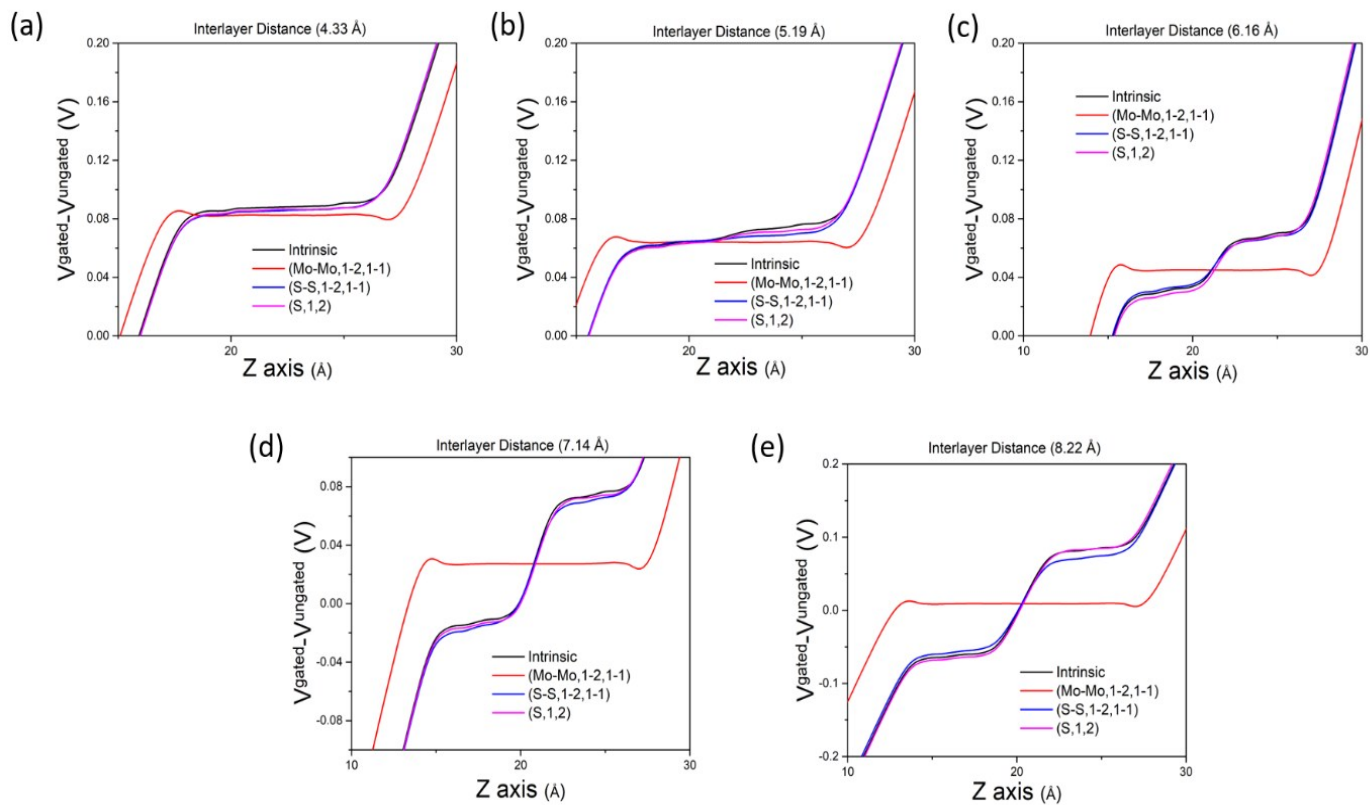

Figure S4: Comparison between the change in potential with and without gate field with 4 different cases Intrinsic, (Mo-Mo,1-2,1-1), (S-S,1-2,1-1) and (S,1,2) with interlayer distances (a) 4.33 Å, (b) 5.19 Å, (c) 6.16 Å, (d) 7.14 Å and (e) 8.22 Å.