Supplementary Information

Fig.S1 shows variation of E_b with R for the considered cases. Zero of R is taken to be the S plane for both hollow and top sites of the monolayer.
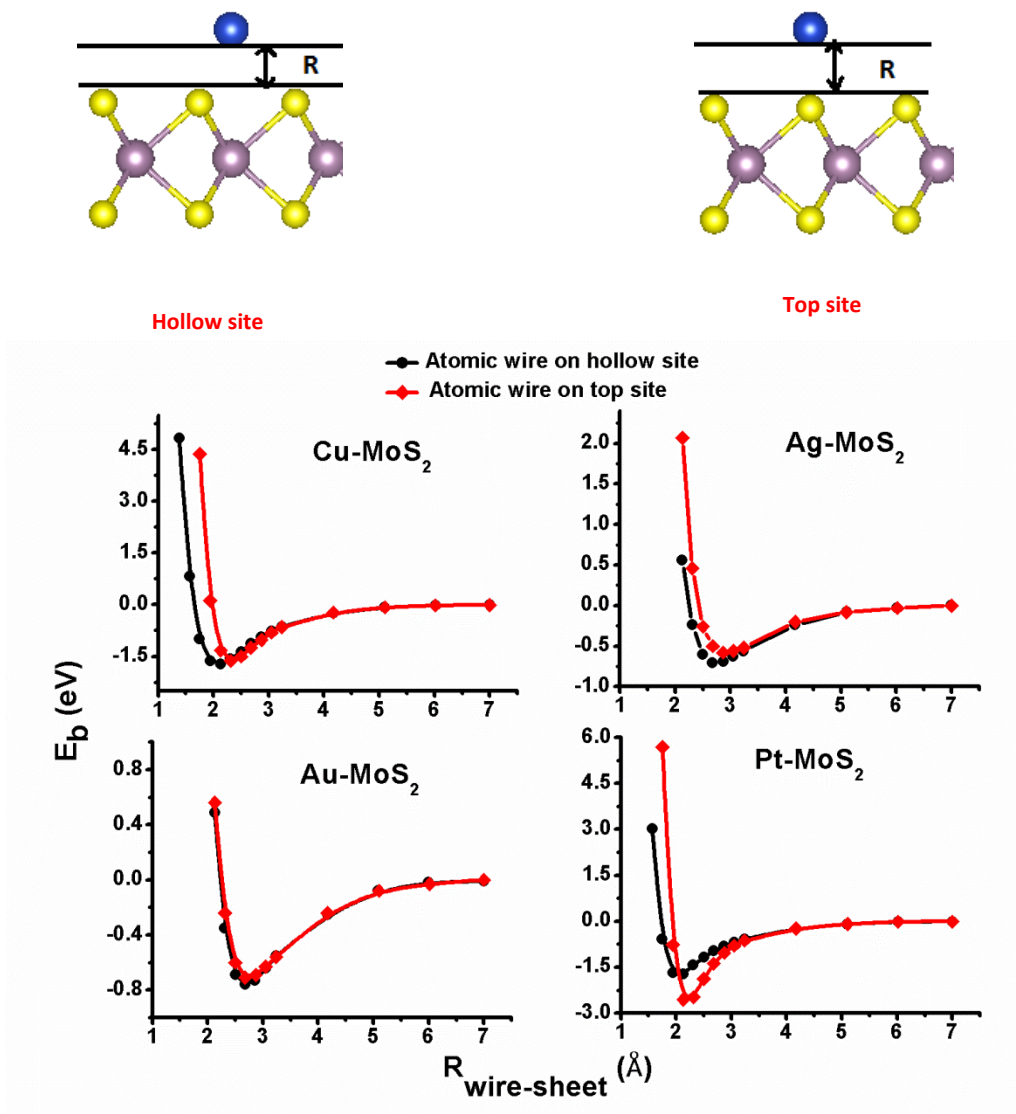

Figure S1: The assembled monolayers: Binding energy (E_b) and distance (R) between wire and monolayer.

A noticeable effect of the lattice mismatch on the binding energy of the wire/monolayer system is seen, though the preferred binding site remains the same (Fig S1); (4x1) Cu wire on (3x3) MoS$_2$ monolayer yields 0.1% lattice mismatch, and the calculated value of E$_b$ for the top site is 0.27 eV/atom (Fig. S2). On the other hand, (5x1) wire on (4x4) monolayer yields 6% lattice mismatch, and E$_b$ for the top site is calculated to be 0.32 eV/atom (Fig S1). Note that positive sign has been used for binding energy value here to make it consistent with the main text of the paper.
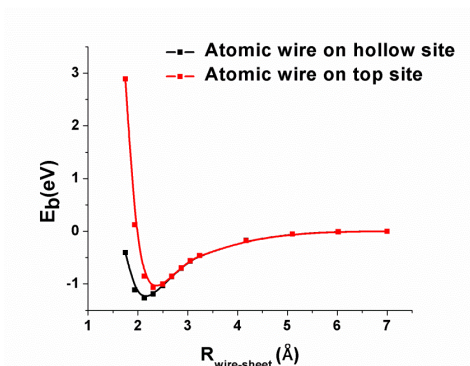
Comment (iv)

Figure S2: Binding energy (E$_b$) and distance (R) between wire and monolayer for the assembled monolayer, (4x1) Cu/(3x3) MoS$_2$.

No difference is also seen for the electronic properties in terms of the band structure and density of states of the assembled monolayer. For example, DOS remains nearly same for the (4x1) Cu/(3x3) MoS_2 and (5x1) Cu/(4x4) monolayer systems. (Fig. S3).
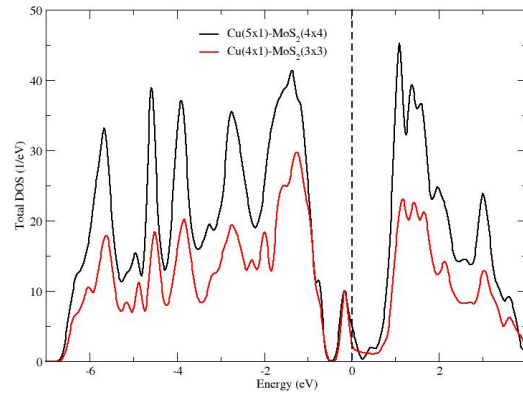

Figure S3: Comparison of total density of states of (4x1) Cu (4x1)/(3x3) monolayer and (5x1) Cu/ (4x4) monolayer systems.
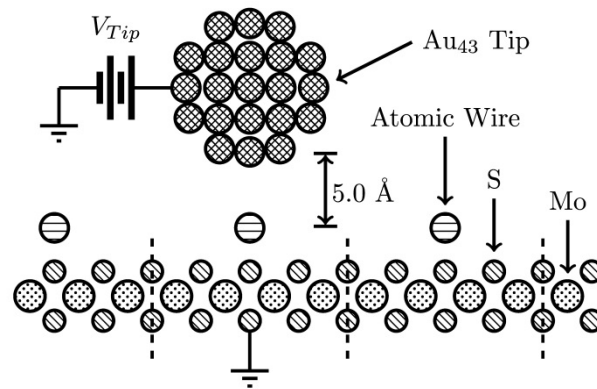

Figure S4: Diagram showing the simulated STM setup. The STM tip is modeled with an Au_{43} cluster, and is separated from the atomic wire/MoS_2 system by 5.0 Angstrom. Three unit cells are depicted, with dashed lines indicating the periodic boundaries.
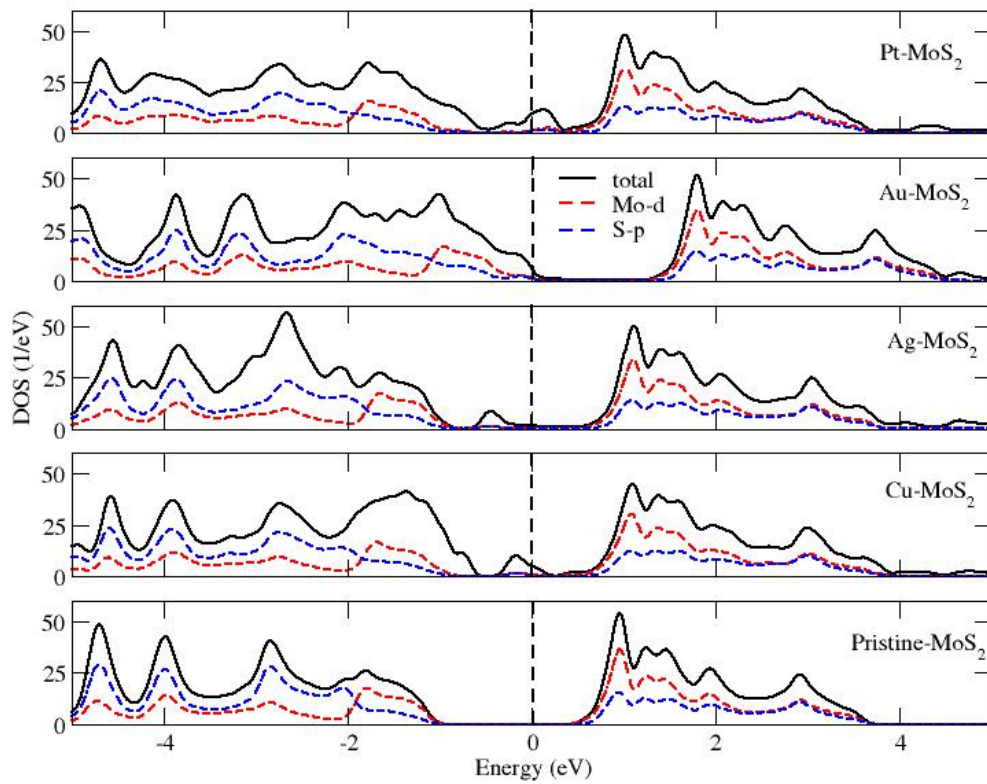
Figure S5: Total and projected density of states of the pristine and assembled MoS_2 monolayers. Zero of the energy is aligned with Fermi energy.