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Supporting Information

Selecting electrode materials for monolayer ReS_2 with Ohmic contact

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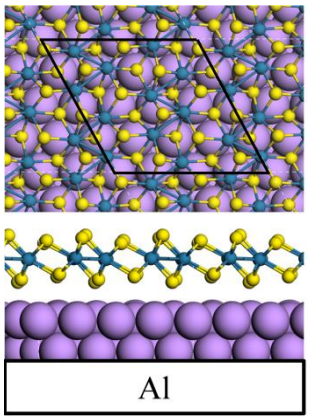

Fig. S1 Top and side views of monolayer $ReSe_2$ on the Al(111) surface. The Al, S and Re atoms are shown in purple, yellow and turquoise colors, respectively. The black box indicates the lateral dimension of supercell.

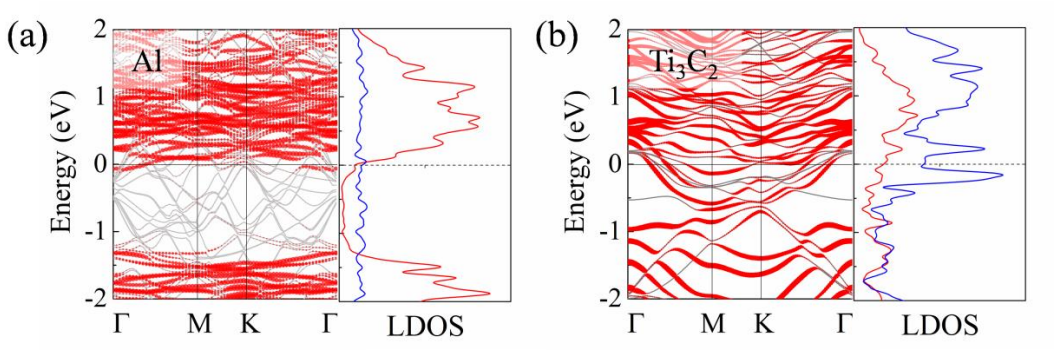

Fig. S2 Left panels: electronic band structures (grey lines) of monolayer ReS_2 on (a) Al(111) surface and (b) Ti_3C_2 MXene. The red lines show the bands from the ReS_2 sheet, and the weight is represented by the line width. Right panels: local density of states (LDOS) from ReS_2 (red lines) and electrode material (blue lines). The Fermi energy is shifted to zero.

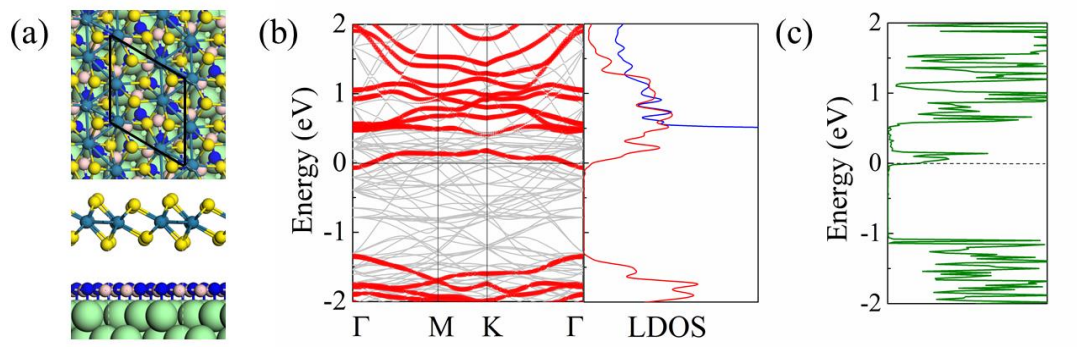

Fig. S3 (a) Top and side views of monolayer $ReSe_2$ on Co/h-BN electrode. The B, N, Co, Se and Re atoms are shown in salmon, blue, green, yellow and turquoise colors, respectively. The black boxes in the top views indicate the lateral dimension of supercell. (b) Left panels: electronic band structures (grey lines) of monolayer ReS_2 on Co/h-BN electrode. The red lines show the bands from the ReS_2 sheet, and the weight is represented by the line width. Right panels: local density of states (LDOS) from ReS_2 (red lines) and electrode material (blue lines). The Fermi energy is shifted to zero. (c) Transmission spectrum at zero bias voltage for the ReS_2 FETs with Co/h-BN electrode. The Fermi energy is shifted to zero. The ReS_2 sheet shows weak coupling with Co/h-BN, having interlayer spacing of 3.39 Å. The band structure and transmission spectrum retain the semiconducting feature of ReS_2 monolayer with band gap and transport gap of 1.24 and 1.04 eV, respectively; both show *n*-type doping character, yielding zero Schottky barriers for electron carriers in the vertical and lateral directions.