Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.


# Hybrid Heterojunctions between a 2D Transition Metal Dichalcogenide and Metal Phthalocyanines: Their Energy Levels vis-à-vis Current Rectification

Arnab Banerjee, Biswajit Kundu, and Amlan J. Pal

Department of Solid State Physics, Indian Association for the Cultivation of Science, Jadavpur, Kolkata 700032, India

E-mail: sspajp@iacs.res.in

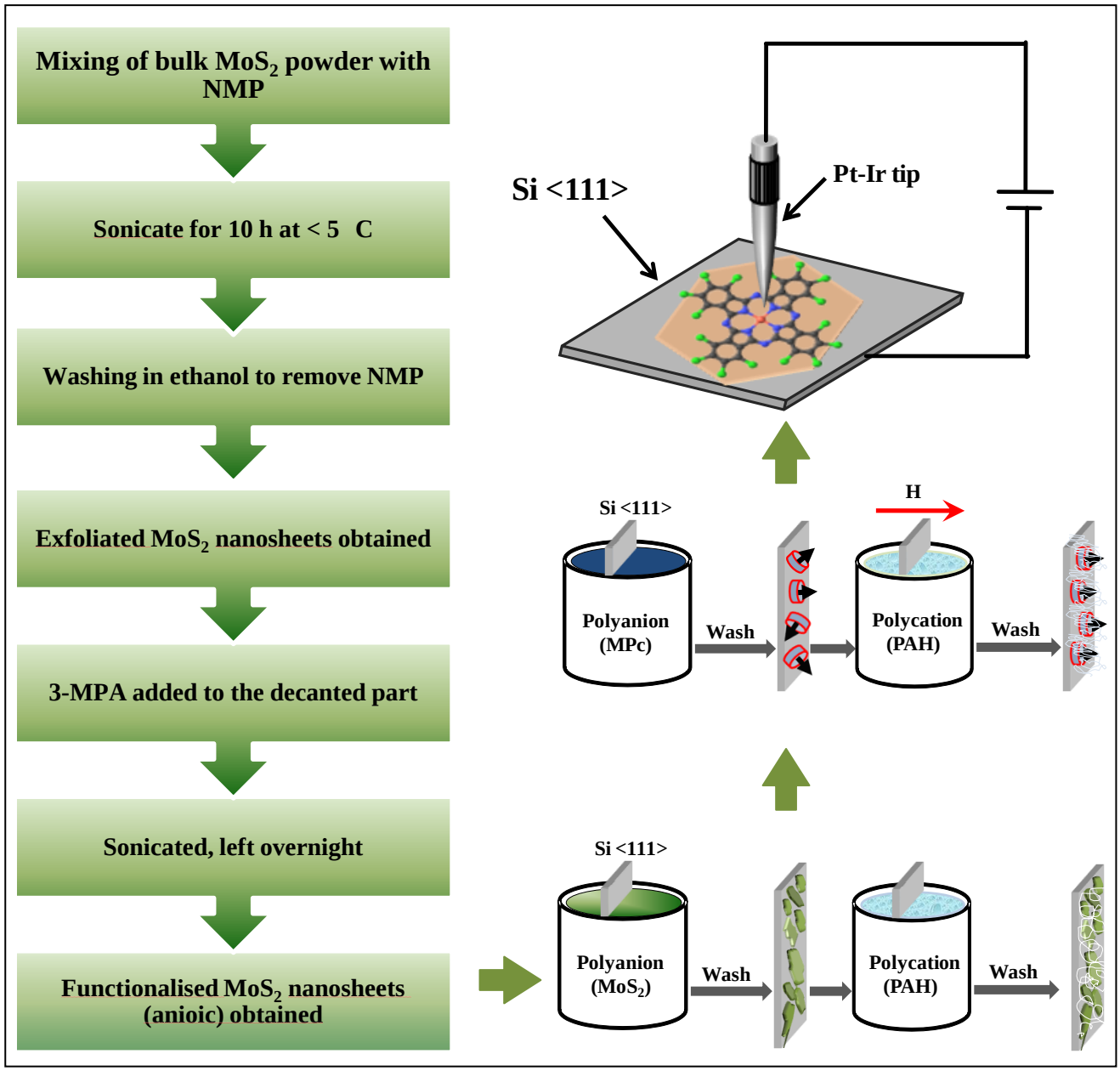


**Fig. S1** Schematic representation of $MoS_2$ exfoliation process, $MoS_2$|MPc heterojunction formation, and their characterization with a STM tip

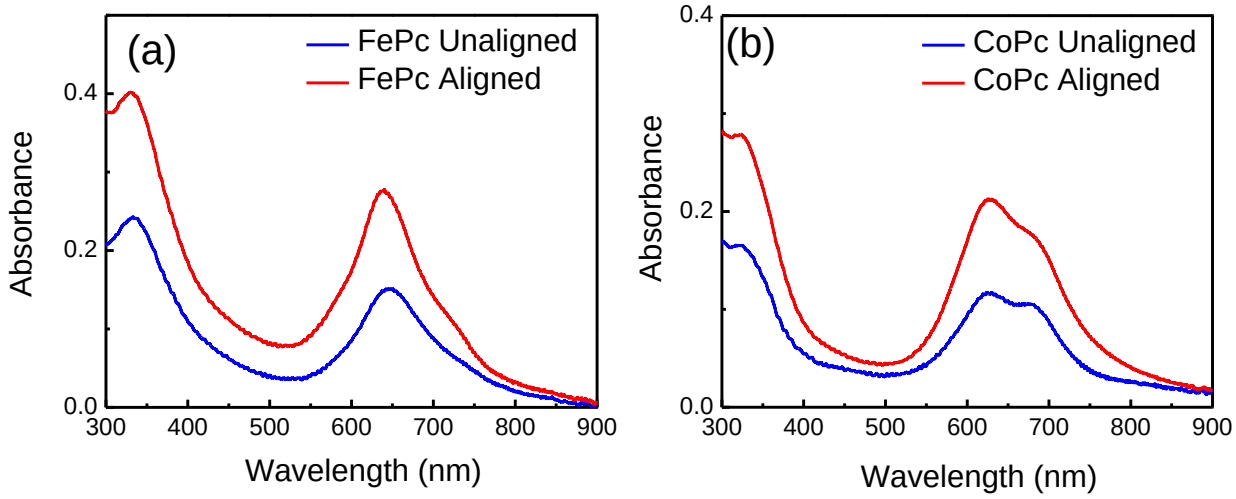


**Fig. S2** Optical absorption spectra of (a) FePc and (b) CoPc (10 bilayers) without and with magnetization vector assistance resulting unaligned and aligned molecules in the LbL films, respectively.

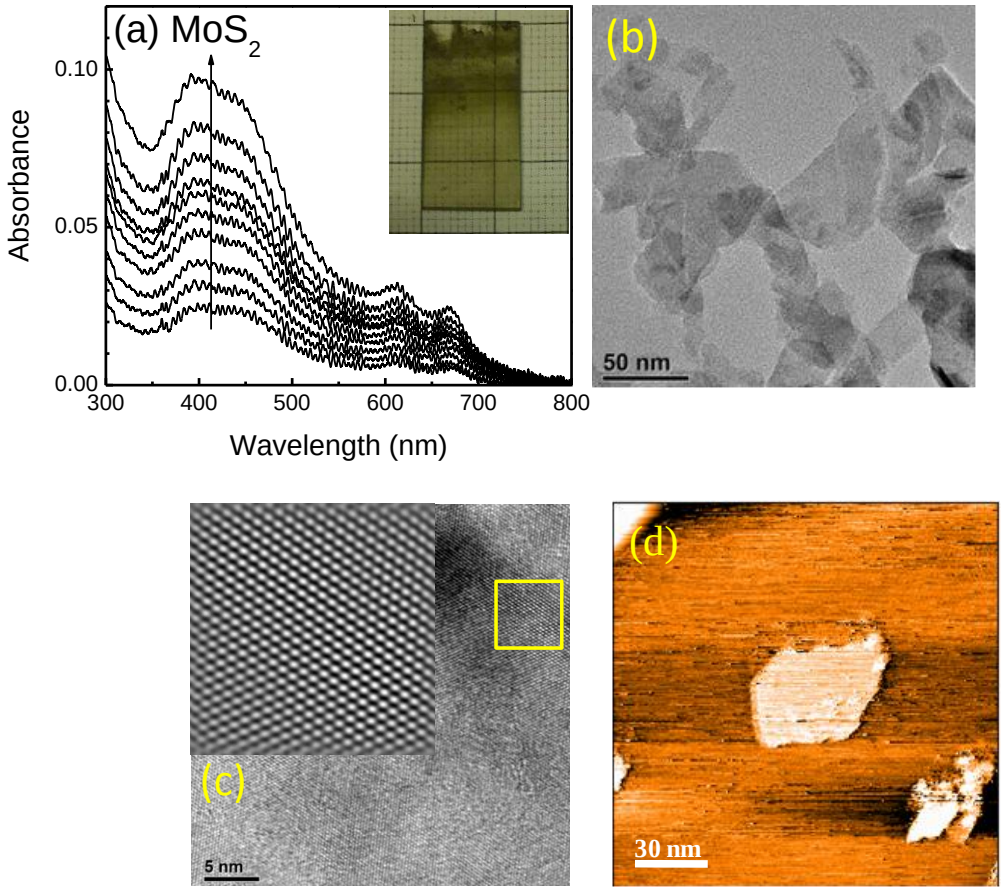


**Fig. S3** (a) Optical absorption spectra of 2D-$MoS_2$ LbL films after adsorption of each bilayer. Arrow indicates the increase in the number of bilayers. Inset shows photograph of around 20-bilayed film deposited on both sides (the upper portion was hold by a clip for LbL deposition). (b) and (c) TEM and HR-TEM images of 2D-$MoS_2$ in its 2H-phase, respectively. (d) STM topography of an exfoliated $MoS_2$ nanosheet. The inset of (c) shows simulated lattice using a software of the squared region.

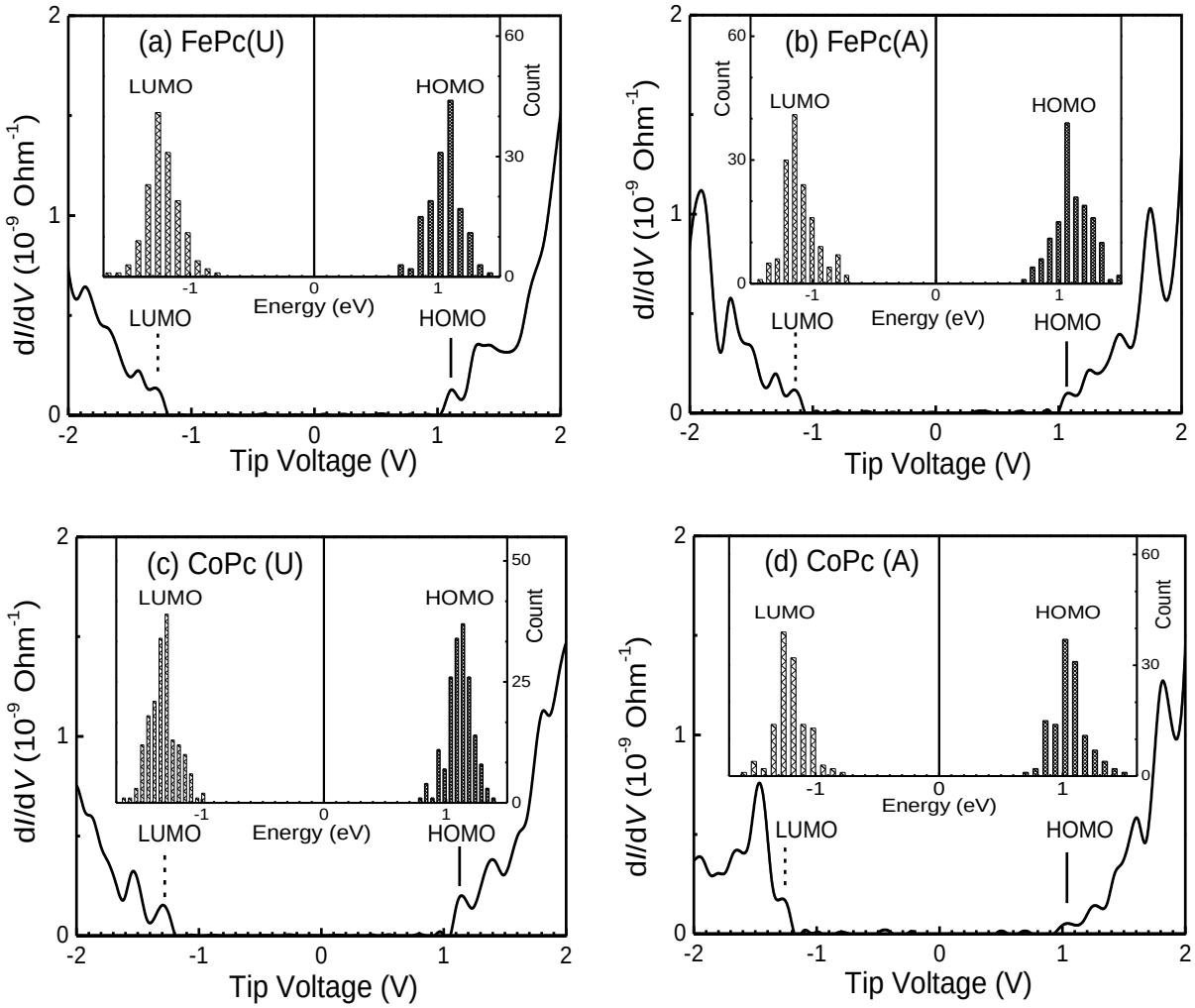


**Fig. S4** A typical differential tunnel conductance spectrum and histogram of HOMO and LUMO energies of FePc in (a) unaligned and (b) aligned forms. In (c)-(d), such a spectrum and histogram of HOMO and LUMO energies of CoPc are shown.

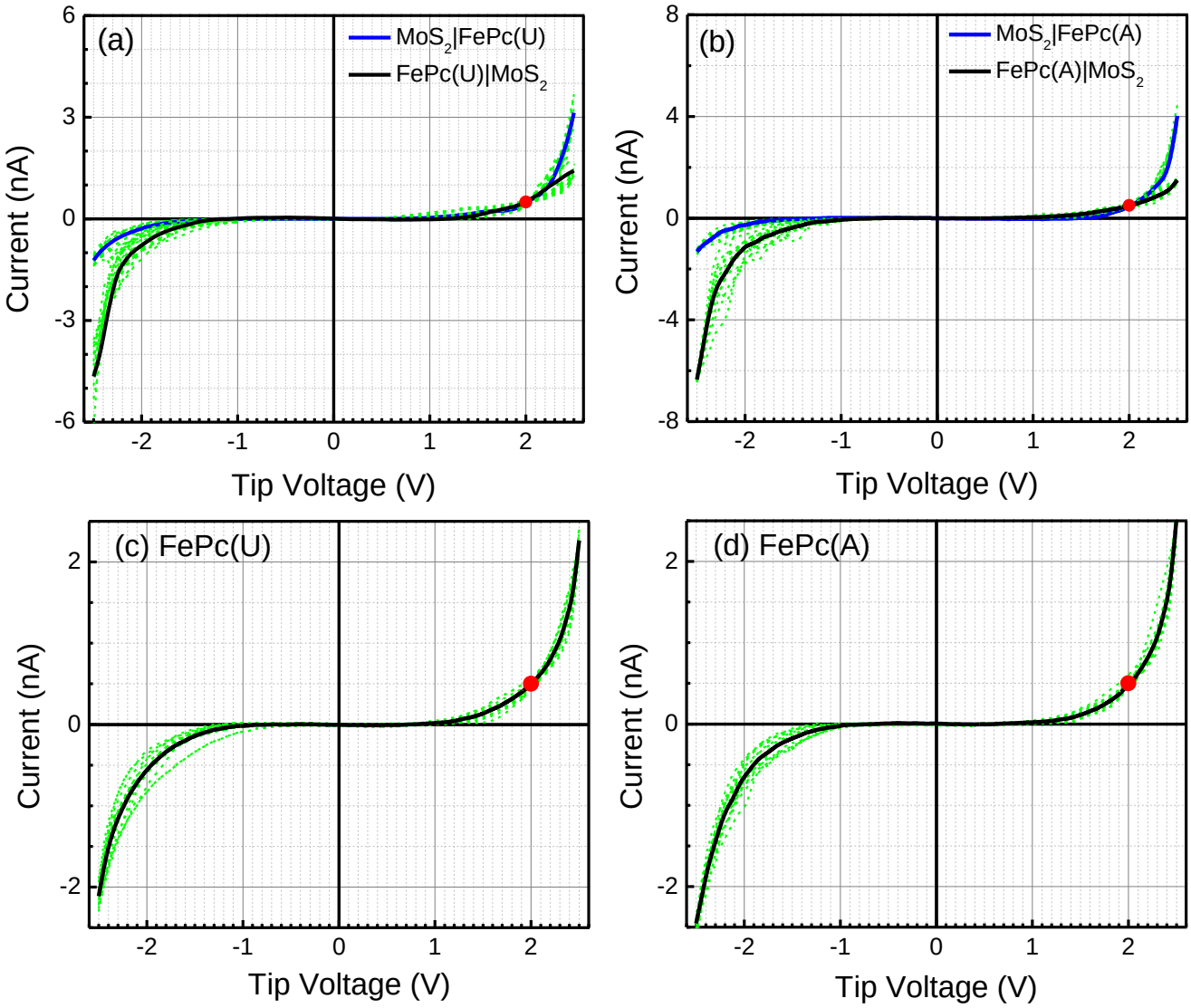


**Fig. S5** (a) Tunneling current versus tip voltage characteristics of FePc(U)|$MoS_2$ junction and its reverse one, $MoS_2$|FePc(U), formed between two monolayers of the semiconductors. (b) Tunneling current versus tip voltage characteristics of FePc(A)|$MoS_2$ and $MoS_2$|FePc(A) junctions. FePc(U) and FePc(A) represented the metal-phthalocyanine in unaligned and aligned forms. Current versus tip voltage characteristics of the components, namely FePc(U), FePc(A) ultrathin-films are shown in (c) and (d), respectively. The set-point of tip-approach has been marked by a red circle in the figures.

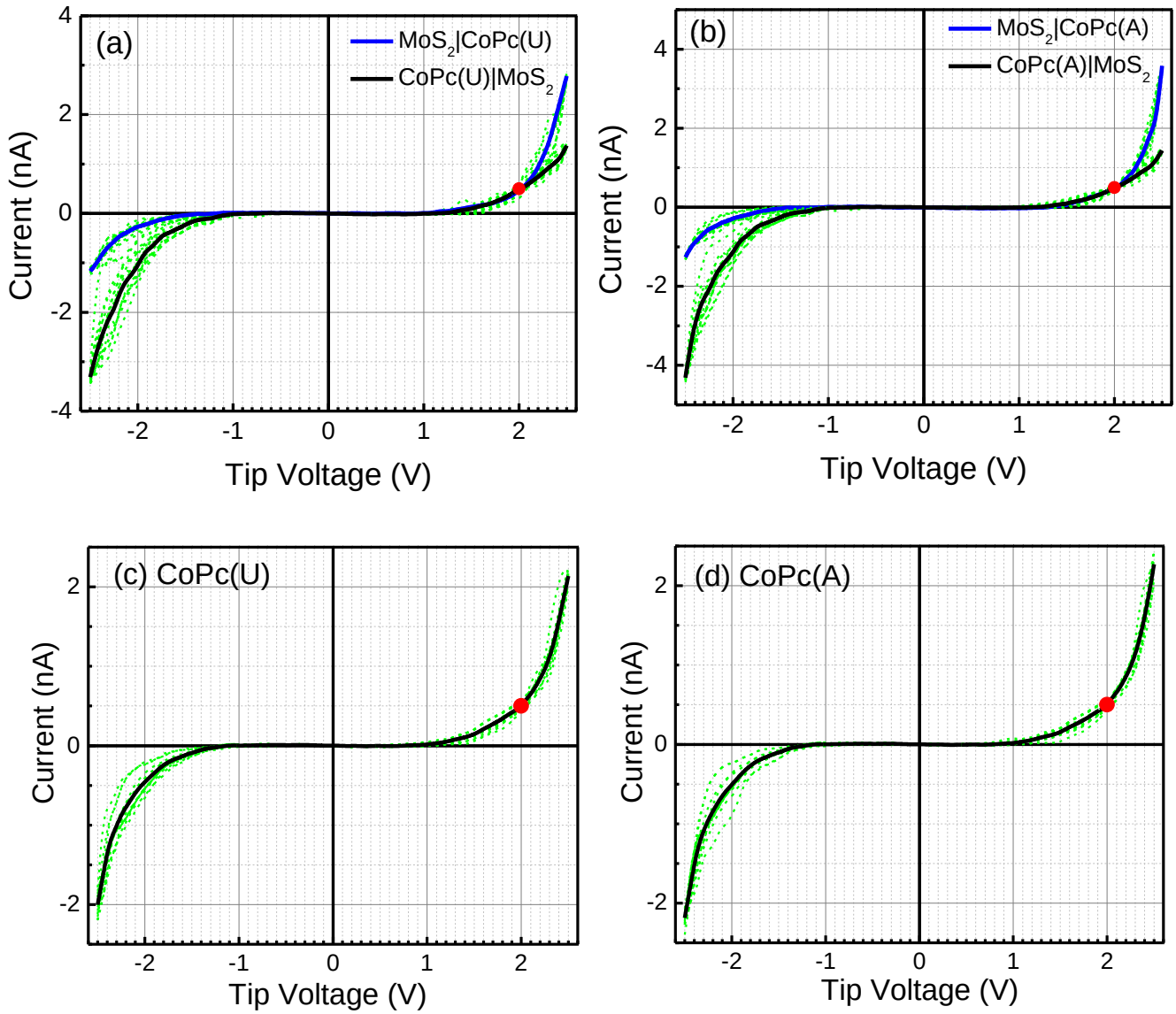


**Fig. S6** (a) Tunneling current versus tip voltage characteristics of CoPc(U)|$MoS_2$ junction and its reverse one, $MoS_2$|CoPc(U), formed between two monolayers of the semiconductors. (b) Tunneling current versus tip voltage characteristics of CoPc(A)|$MoS_2$ and $MoS_2$|CoPc(A) junctions. CoPc(U) and CoPc(A) represented the metal-phthalocyanine in unaligned and aligned forms. Current versus tip voltage characteristics of the components, namely CoPc(U), CoPc(A) ultrathin-films are shown in (c) and (d), respectively. The set-point of tip-approach has been marked by a red circle in the figures.