Supplementary Material

Spin-transfer-torque mediated quantum magnetotransport in MoS_2/Phosphorene vdW Heterostructure based MTJs

Sushant Kumar Behera and Pritam Deb*
Advanced Functional Material Laboratory (AFML), Department of Physics, Tezpur University (Central University), Tezpur-784028, India.
*Corresponding author
Email address: pdeb@tezu.ernet.in (Pritam Deb)

NEGF Formalism

Within the NEGF-DFT framework, we use the self-energy form in the retarded Green's function where, $w_L^{'} = \begin{pmatrix} w_L & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ and $w_R^{'} = \begin{pmatrix} w_R & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ are the co-efficient to present the left and right lead region. In this DFT simulation with plain wave basis, '*w'* would be calculated in the orbital space.

$$w_{\mu\vartheta} = \int dr \text{ב}_{\mu}^{*}(r) w(z) \text{ב}_{\vartheta}(r)$$

Where, $\text{ב}_{\mu(\vartheta)}$ is the atomic basis set and w(z) is defined in the real space.

$$w(z) = \frac{\hbar^2}{2m}\left(\frac{2\pi}{\Delta m}\right)^2 f(z)$$

Here, $\Delta z = z_1 - z_2$ is the length of the scattering region with z_1 and z_2 are the starting and ending points, respectively of each lead along the transport direction z.

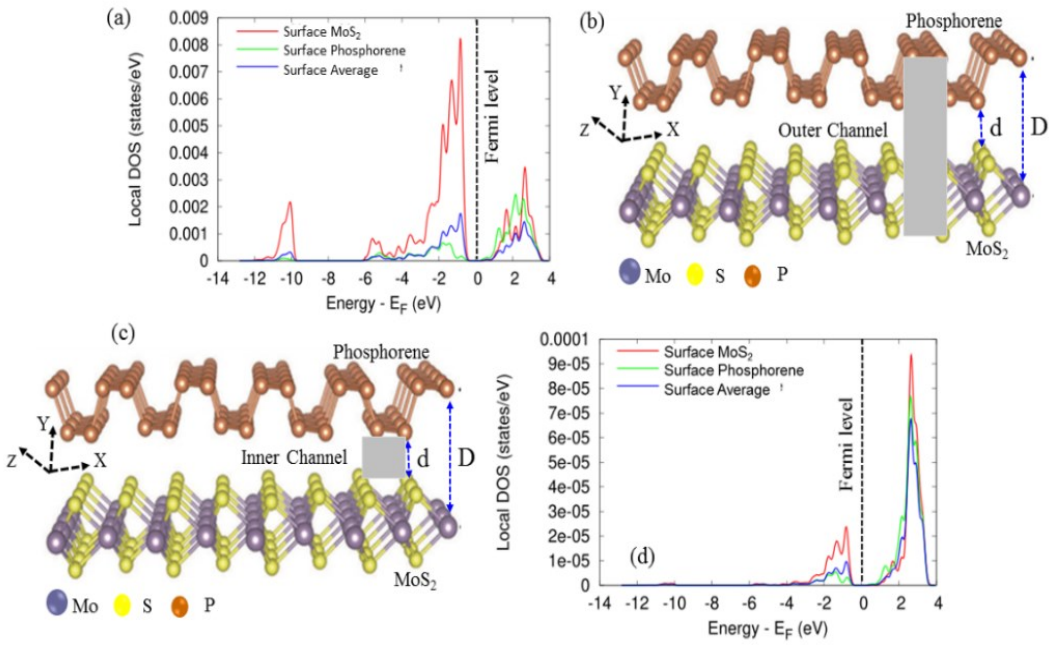

Figure S1. Density of states for surface of the monolayer along with local states of the bilayer (a) where the first vacuum level is localized in (b). Similarly, the DOS pattern of the systems (c) and corresponding second vacuum level (d) have been shown.

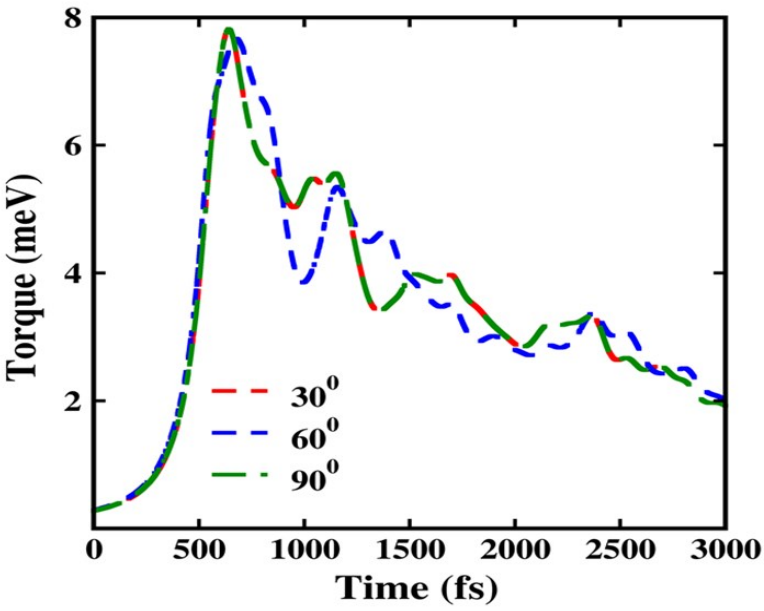

Figure S2. Time-dependent spin-current induced STT of Fe/MoS_2-P/Pt layers under positive bias of 30 mV with different θ.