Annexure B

Detailed description of inset images

This section will describe all the inset images in the chapters with enhanced visibility and extensive detail.

B.1 Energy Vs Transmission Plot

This section will cover the transmission plot as a function of energy as described in fig. 4.3 (a & b).

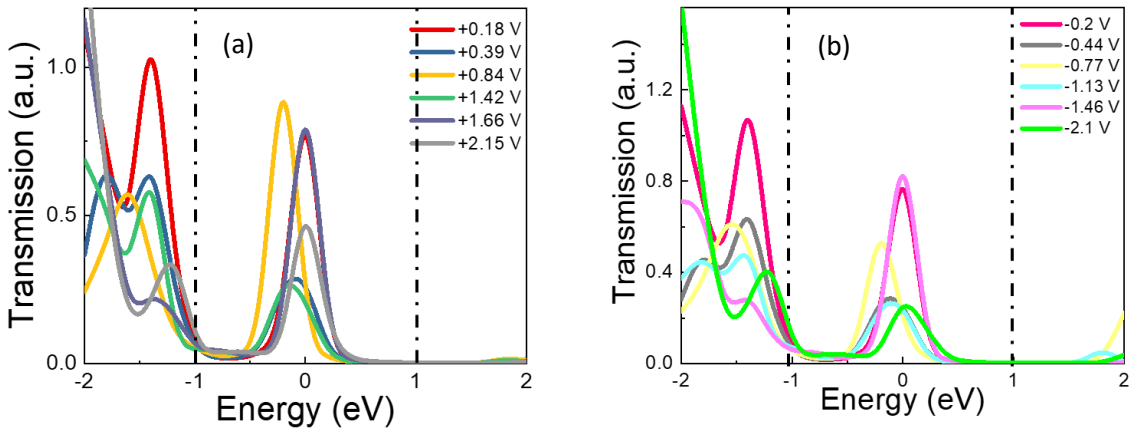

Fig.B1 (a) Transmission spectrum as a function of energy corresponding to peak and valley voltages along positive biasing. (b) Transmission vs energy plot for individual peak and valley voltages in negative biasing.

B.2 Conductance Plot of singly and doubly reduced DDQ

This section will show the effect of reduction on the conduction plot of the DDQ molecule. The conductance plot of doubly reduced DDQ molecule shows additional features as compared to that of singly reduced molecule. See inset images in fig. 4.6.

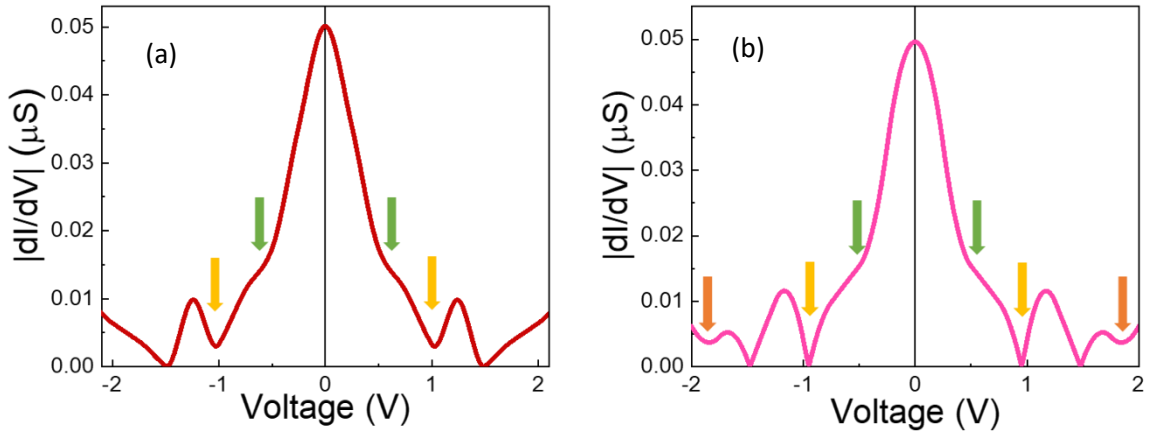

Fig.B2 (a) Conductance Plot of singly reduced DDQ molecule device. The green arrows correspond to shoulder while yellow arrows pointed towards local conductance minima. (b) Conductance plot of doubly reduced DDQ molecule device the orange arrows pointed towards additional feature coming into picture due to double reduction.

B.3 Schematic of DDQ molecule on gold substrate

This section will cover top, side and front view schematics of a normally horizontal DDQ molecule and compare same views for a 30° tilted molecule.

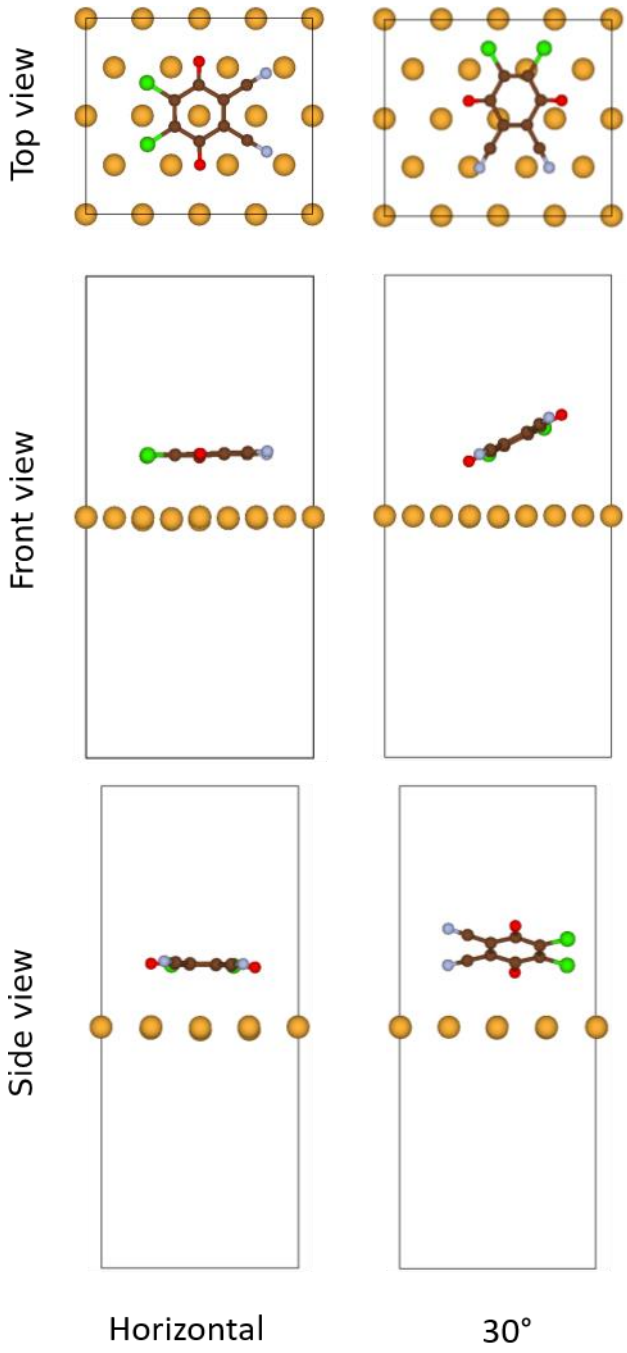

Fig.B3 The schematic representation of various views of DDQ molecule laying on gold substrate horizontally as well as with a 30° tilt.

B.4 Simulated and experimental profiling of DDQ molecule

This section illustrates the profiling plot of DDQ molecule simulated using VASP package and compression with STM data for both horizontal as well as 30° tilted molecule.

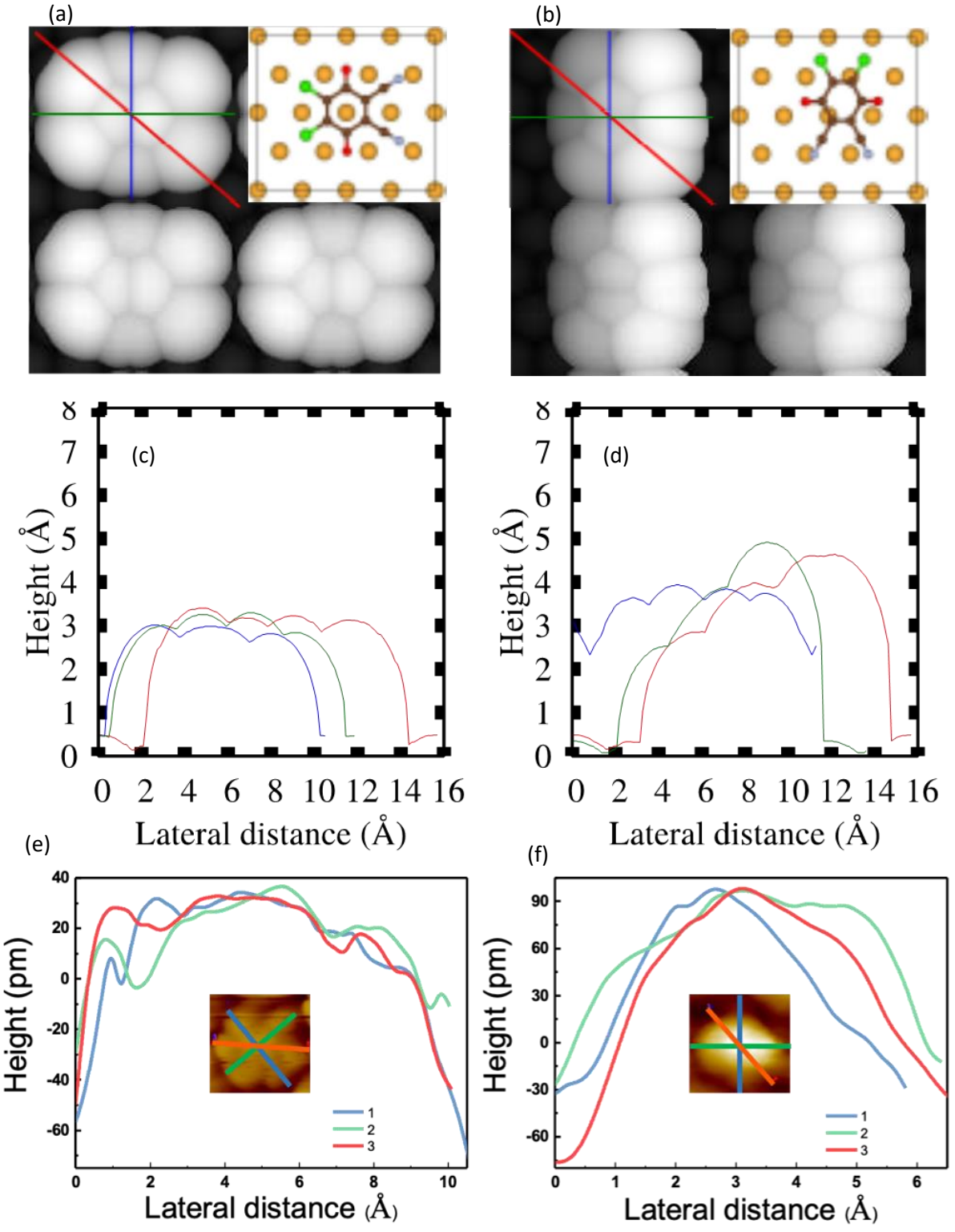

Fig.B4 (a) The simulated micrograph of horizontally laying DDQ molecules on gold substrate using VASP package. (b) Simulated image of DDQ molecule's self-assembly at a tilt angle of 30°. (c) Line profile of simulated horizontally laying DDQ molecule. (d) corresponding line profiling for a 30° tilted DDQ molecule. (e-f) The experimentally obtained line profile of both horizontally laying and tilted 30° on gold 111 substrate using STM.

B.5 Average conductance plot of DDQ molecule

This section describes the average conductance and absolute average conductance plot. The conductance plot helps us to identify frontier orbitals as well as zero cross over signifies negative differential resistance (NDR) behavior of the molecule.

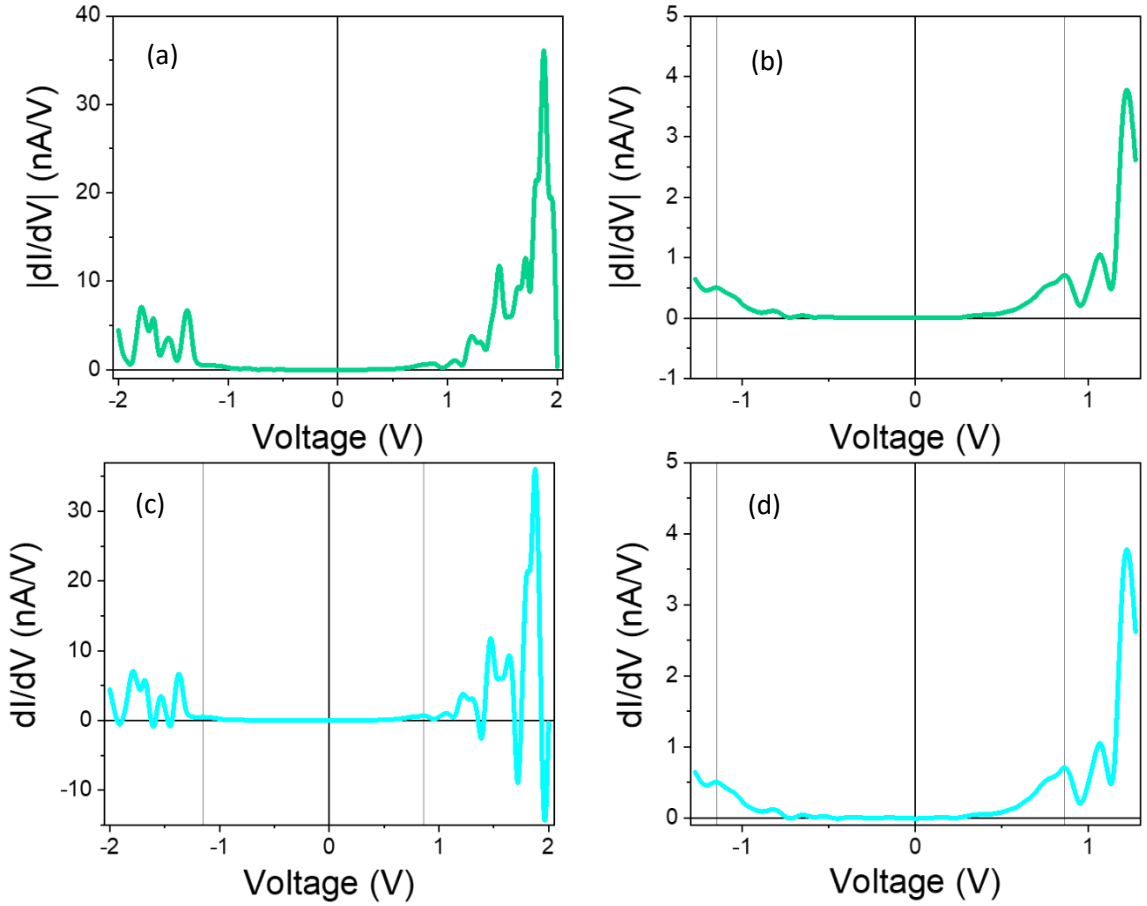

Fig.B5 (a) The absolute valued conductance vs voltage plot. (b) zoomed in section to emphasize on frontier orbitals. (c-d) The averaged conductance plot with multiple zero crossovers along with zoomed section with frontier orbital at -1.15V and 0.86V.

B.6 Plot of translation slope vs voltage

This section explains the plot of translational slope along voltage. The translational slop is essentially account for change in coordinate values with every step voltage.

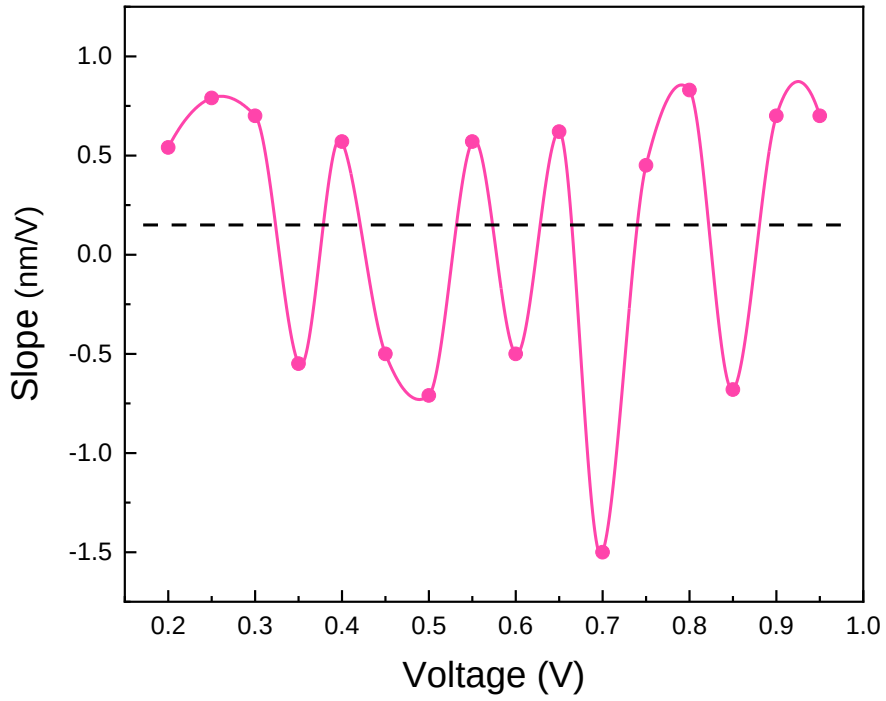

Fig.B6 The plot depict an oscillatory relation between translation slope and tip biasing.