

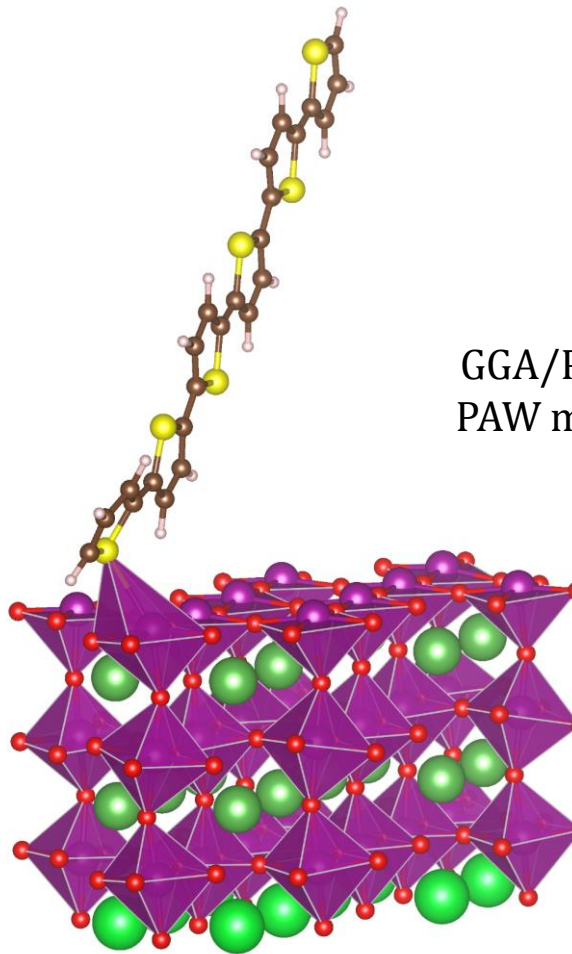
Ab-initio design of the spinterface based on α -sexithiophene/ LSMO

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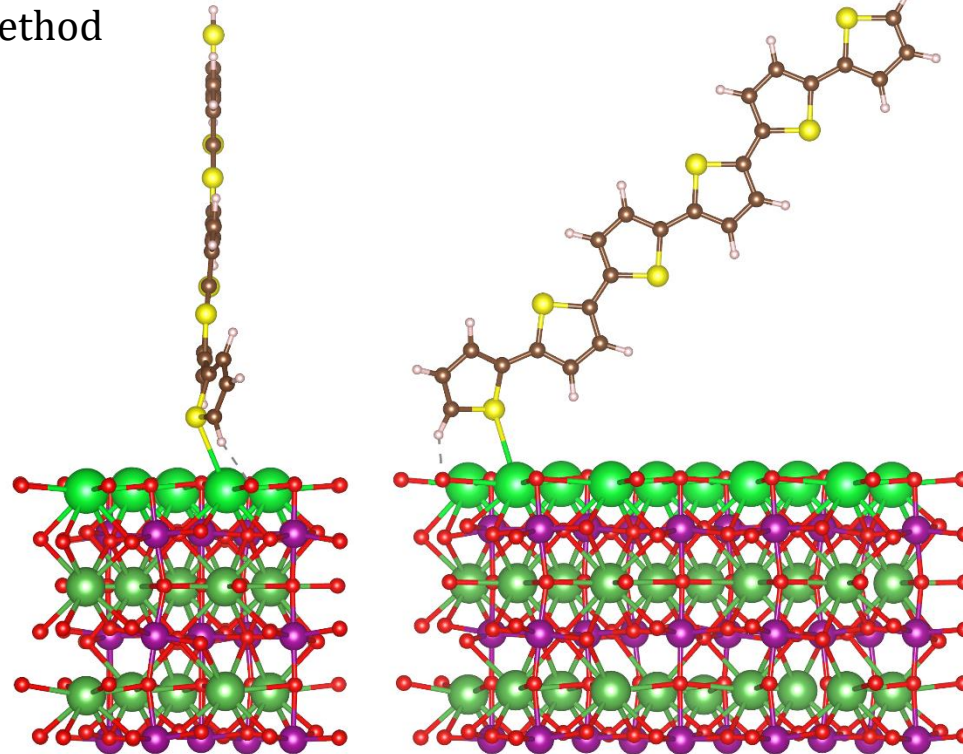


GGA/PBE+U
PAW method



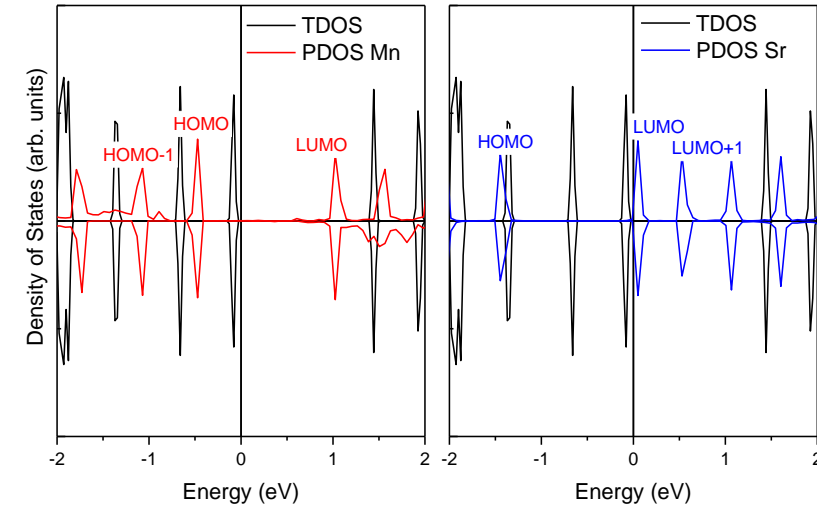
**LSMO/T6 (MnO)
heterostructure**

Mn, O, La, Sr, C, and S atoms are depicted in purple, red, green, neon, brown, and yellow, respectively



LSMO/T6 (SrO) heterostructure

Mn, O, La, Sr, C, and S atoms are depicted in purple, red, green, neon, brown, and yellow, respectively



**Comparison of TDOS of
free-standing 6T
molecule with PDOS of
adsorbed 6T**

TDOS of free-standing 6T molecule in black, PDOS of 6T adsorbed on Mn-O surface in red (left). (Right) with PDOS of 6T adsorbed on Sr-O surface in blue.