Electronic Supplementary Material (ESI) for Nanoscale.

Single atom alloy catalyst for SO_3 decomposition: Enhancement of platinum catalyst`s performance by Ag atom embedding

Sandeep Nigam* and Chiranjib Majumder

Supporting Information

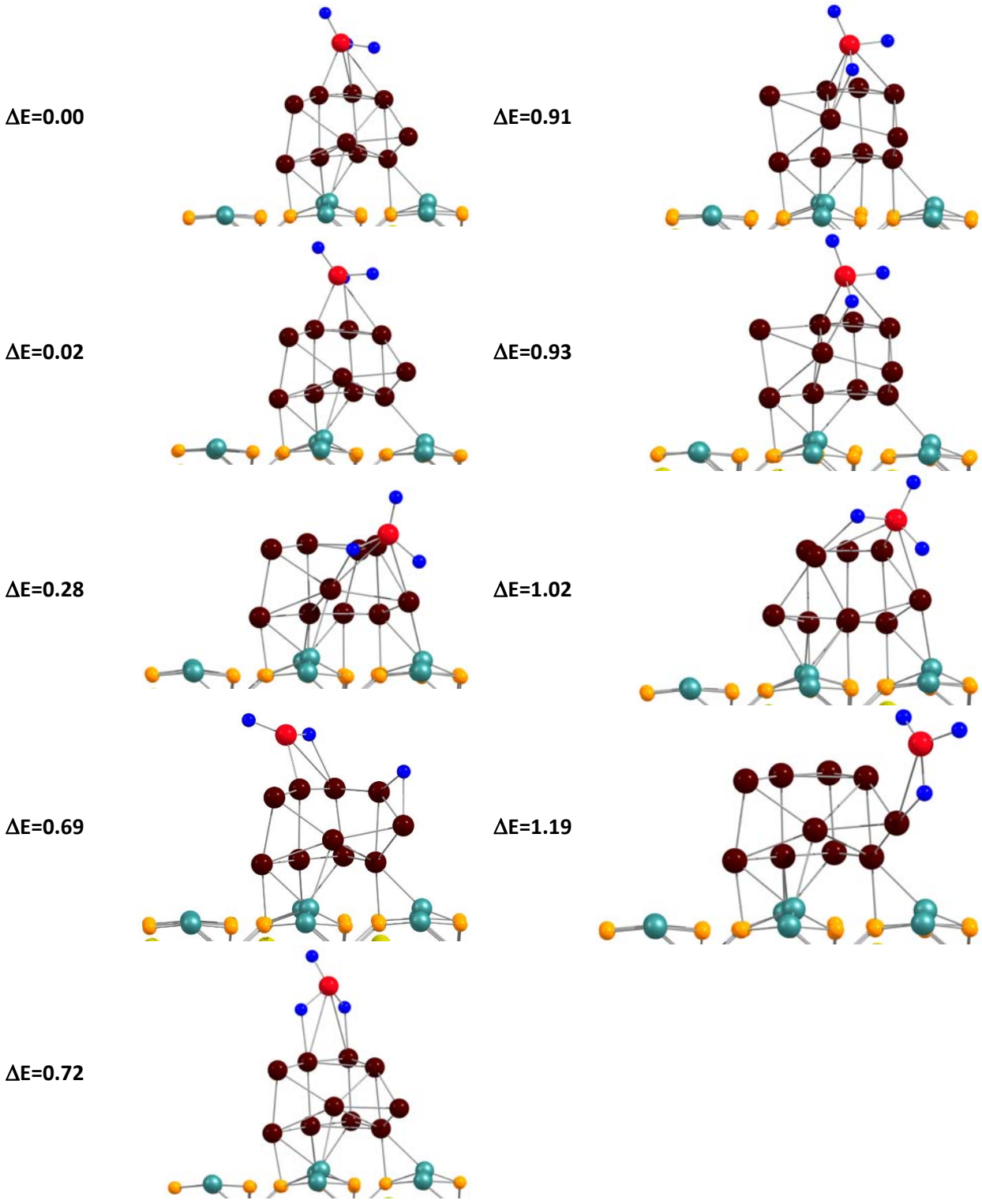


Figure-S1: Low lying isomer of SO_3-(Pt_{10}@Al_2O_3) complex. ΔE indicates relative stability.

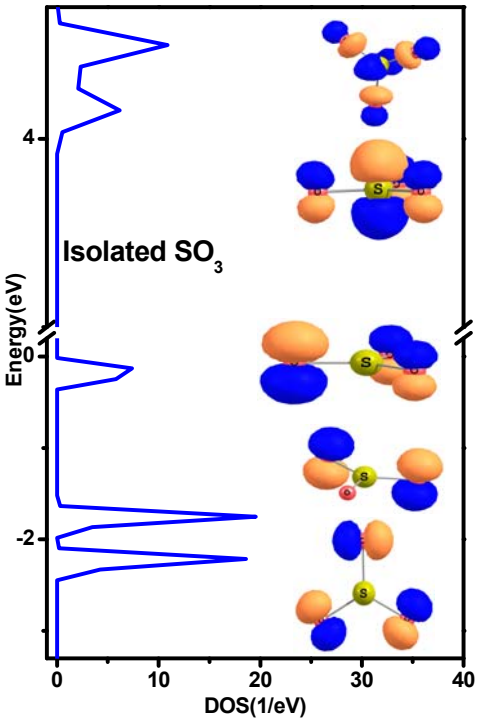


Figure-S2: Electronic density of states of pristine SO_3 molecule. Molecular Orbital pictures has been obtained via all electron calculations at B3LYP/6-311+g(d, p) level of theory.

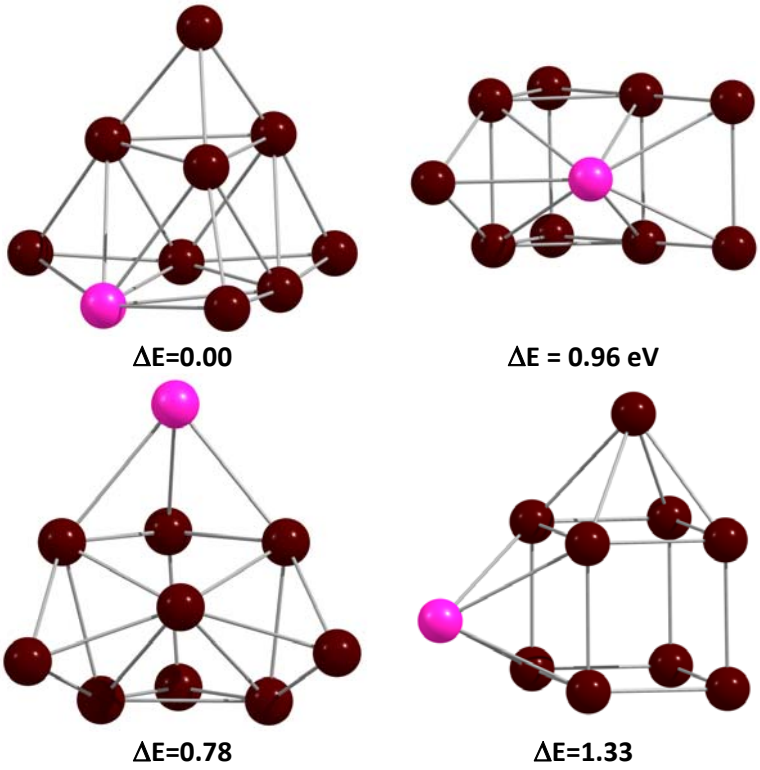


Figure-S3: Low lying isomer of gas phase $AgPt_9$ cluster. ΔE indicates relative stability.

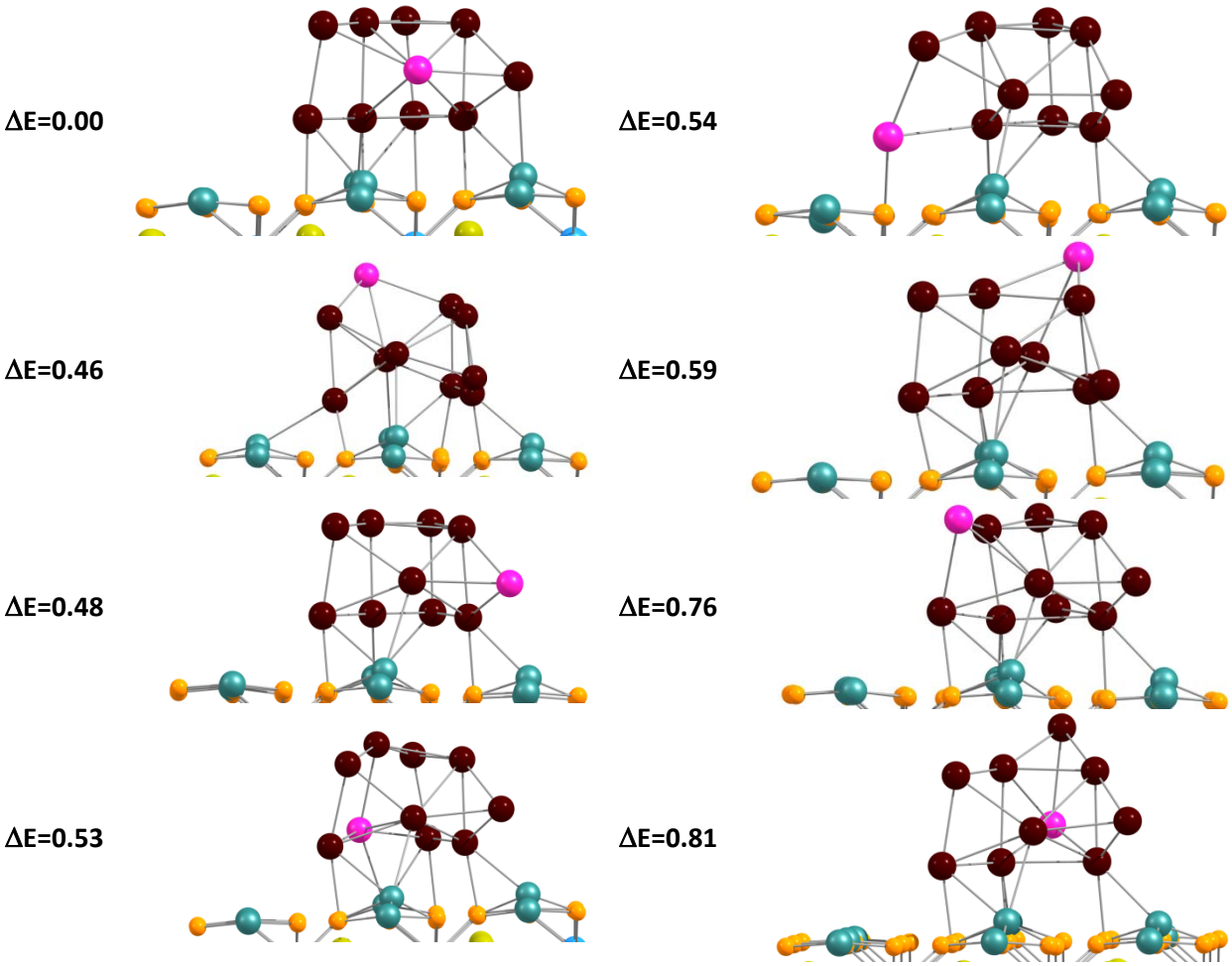
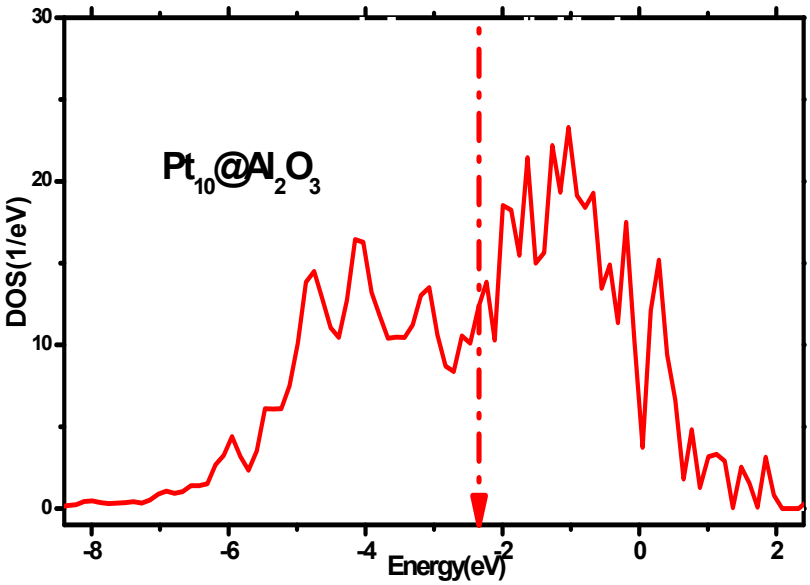


Figure-S4: Low lying isomer of $AgPt_9@Al_2O_3$) cluster. ΔE indicates relative stability.

(a)

$Pt_{10}@Al_2O_3$
d-band centre
-2.36 eV



(b)

$AgPt_9@Al_2O_3$
d-band centre
-2.27 eV

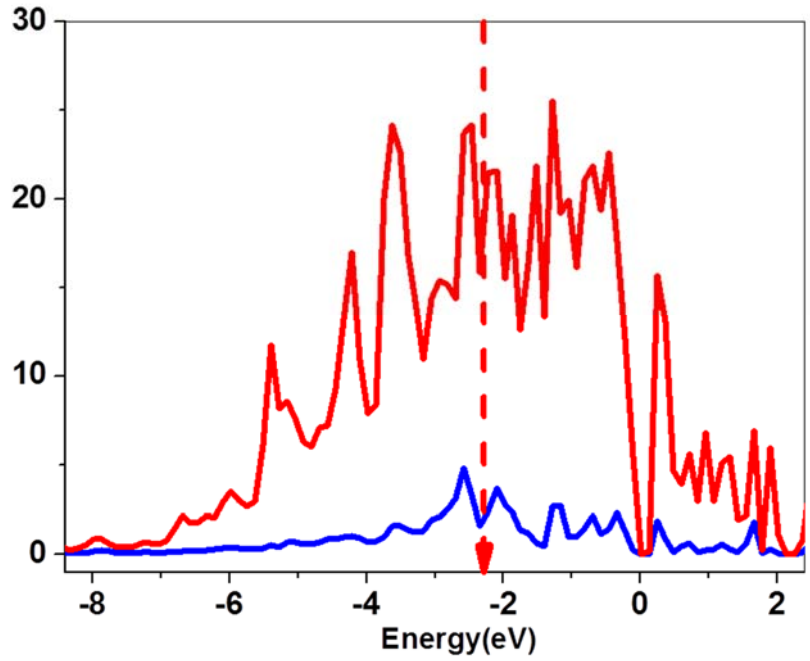


Figure-S5: Comparative DOS spectrum of (a) $Pt_{10}@Al_2O_3$ and (b) $AgPt_9@Al_2O_3$.

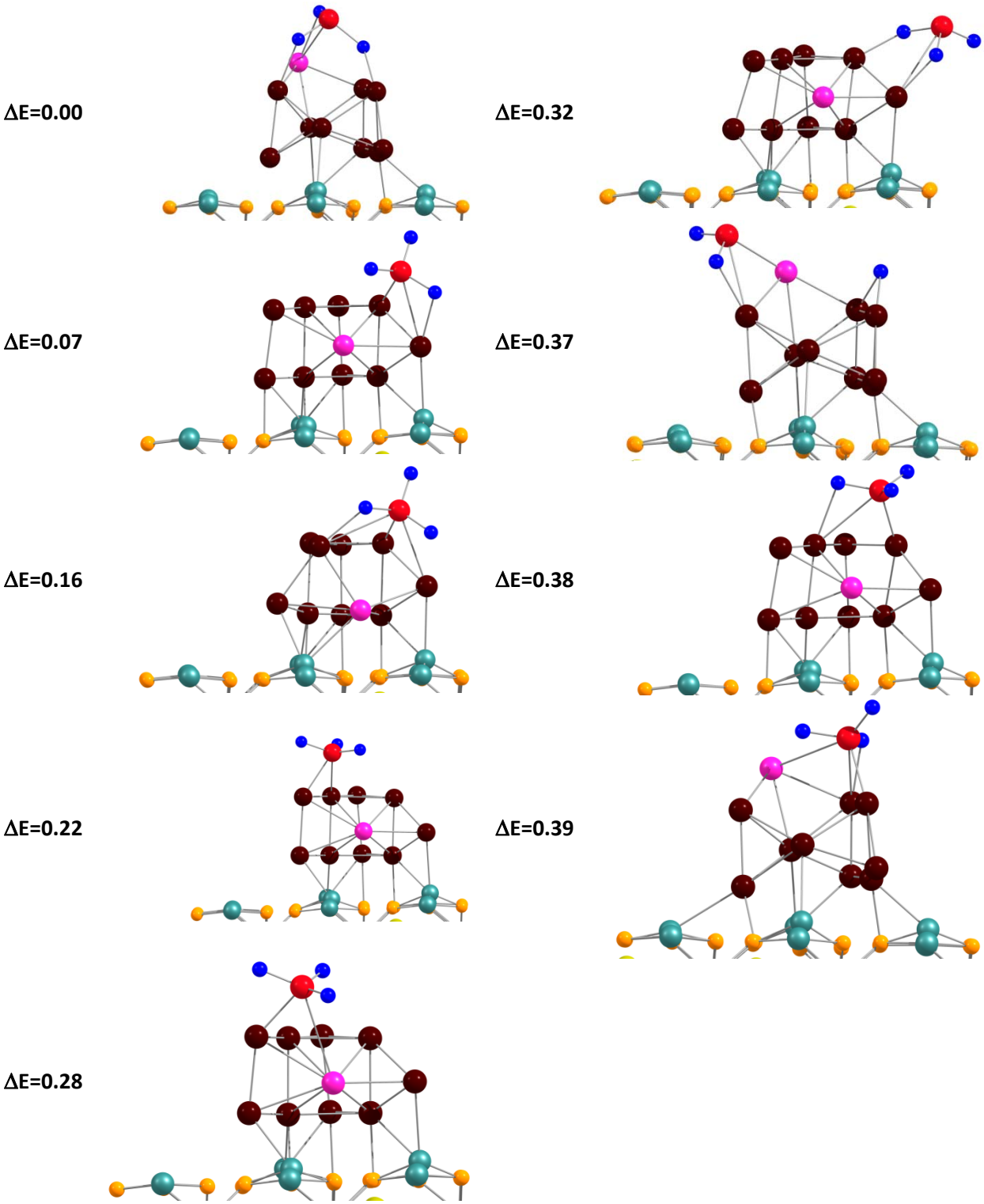


Figure-S6: Low lying isomer of SO_3-($AgPt_9$@Al_2O_3) complex. ΔE indicates relative stability.

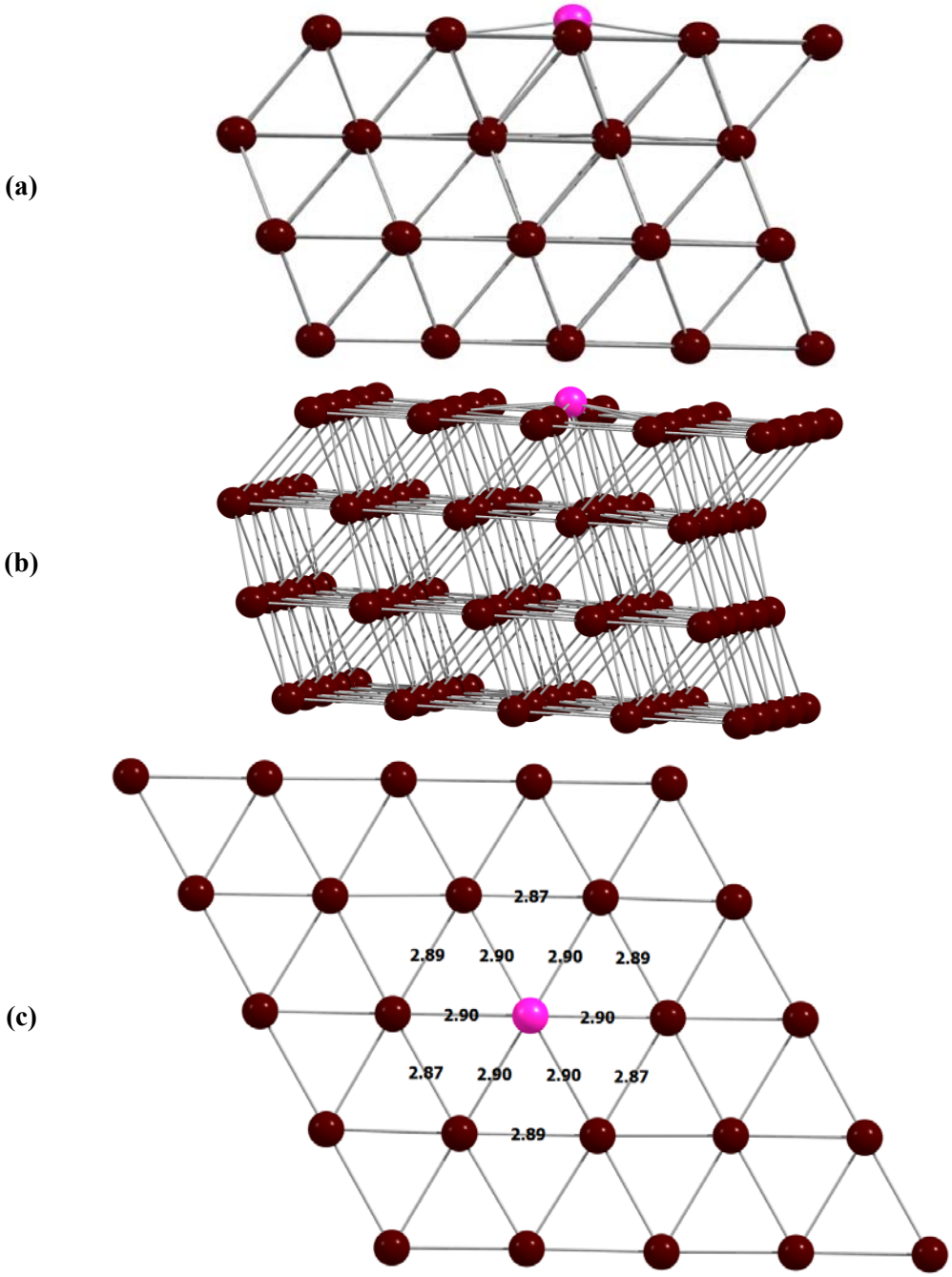


Figure-S7: Single Ag atom substituted Pt(111) surface. The substitution at 2nd and 3rd layer is found to be 0.25 and 0.26 eV higher in energy.

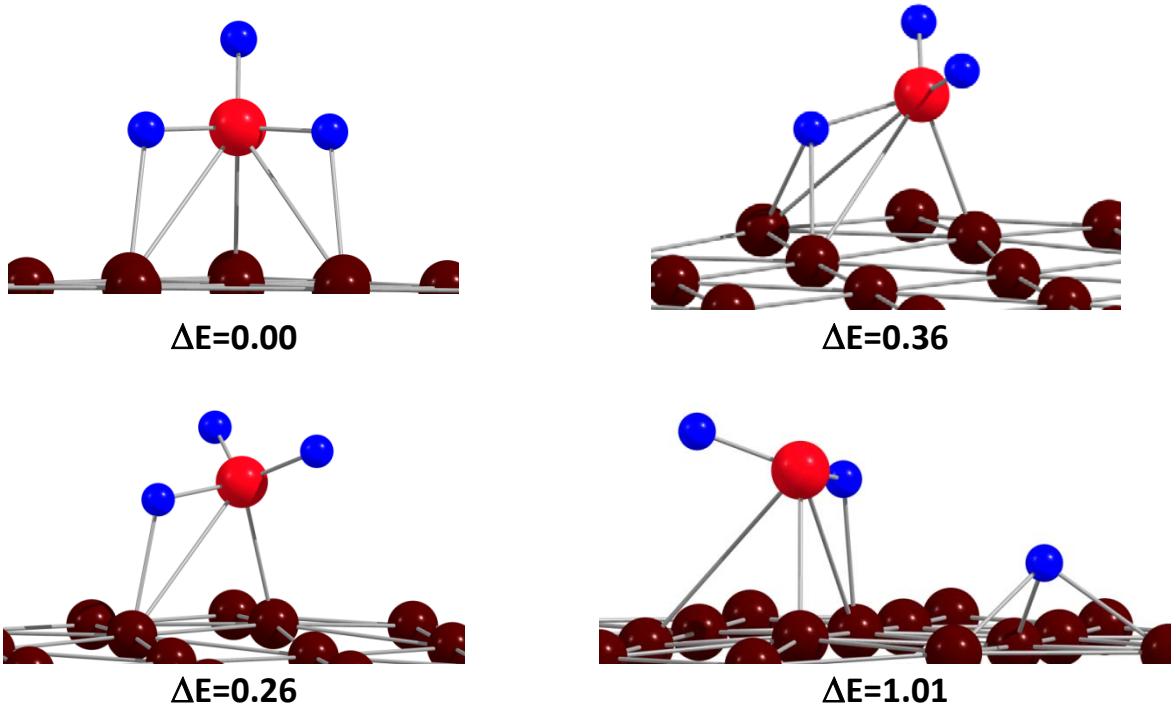


Figure-S8: Low lying isomer of SO_3 on Pt(111) and $Ag_1Pt(111)$ surface. ΔE indicates relative stability.