

“Supporting Information”

NO reduction over Al-embedded MoS₂ monolayer: A first-principles study

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Figure S1. The energy diagram and optimized stationary points for the diffusion of the Al atom on defective MoS₂

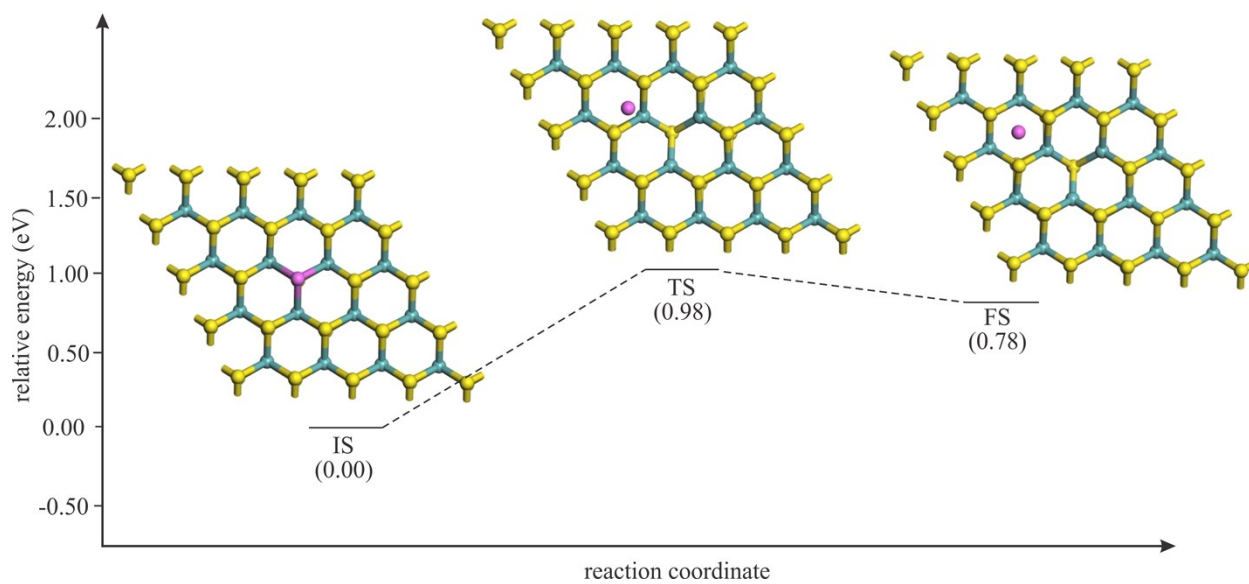


Figure S2. The frontier molecular orbitals of isolated NO and CO molecules

