



S1. Charge transfers at Fe@G and Fe by the adsorptions of (a) NO and (b) NO₂. The blue and yellow surfaces present the charge depletions and accumulations with -0.002 and 0.002 $e/\text{\AA}^3$ iso-values, respectively. The charge transfer aspects, depletions of spin-majority charge from Fe and Fe@G are similar with those of Co and Co@G.