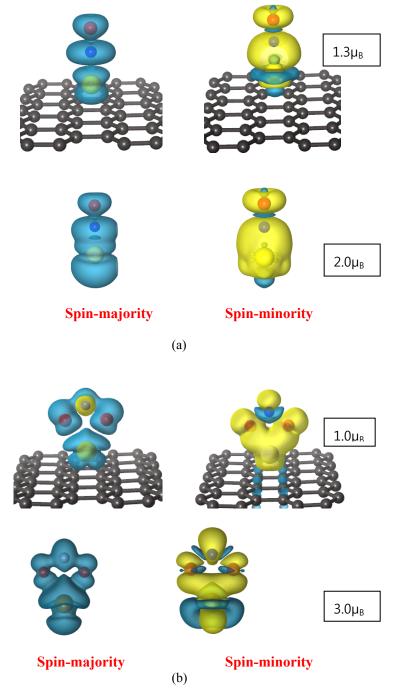
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S1. Charge transfers at Fe@G and Fe by the adsorptions of (a) NO and (b) NO₂. The blue and yellow surfaces present the charge depletions and accumulations with -0.002 and 0.002 $e/\text{Å}^3$ iso-values, respectively. The charge transfer aspects, depletions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