

**Carbon dioxide interaction with isolated imidazole or attached on gold
clusters and surface: competition between σ H-bond and π stacking
interaction**

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Supplementary material

Figure S1: Electron density surface (isosurface value 0.02 a.u) of $Im@Au_{20}$ (left) and $Im@Au(111)$ (right).

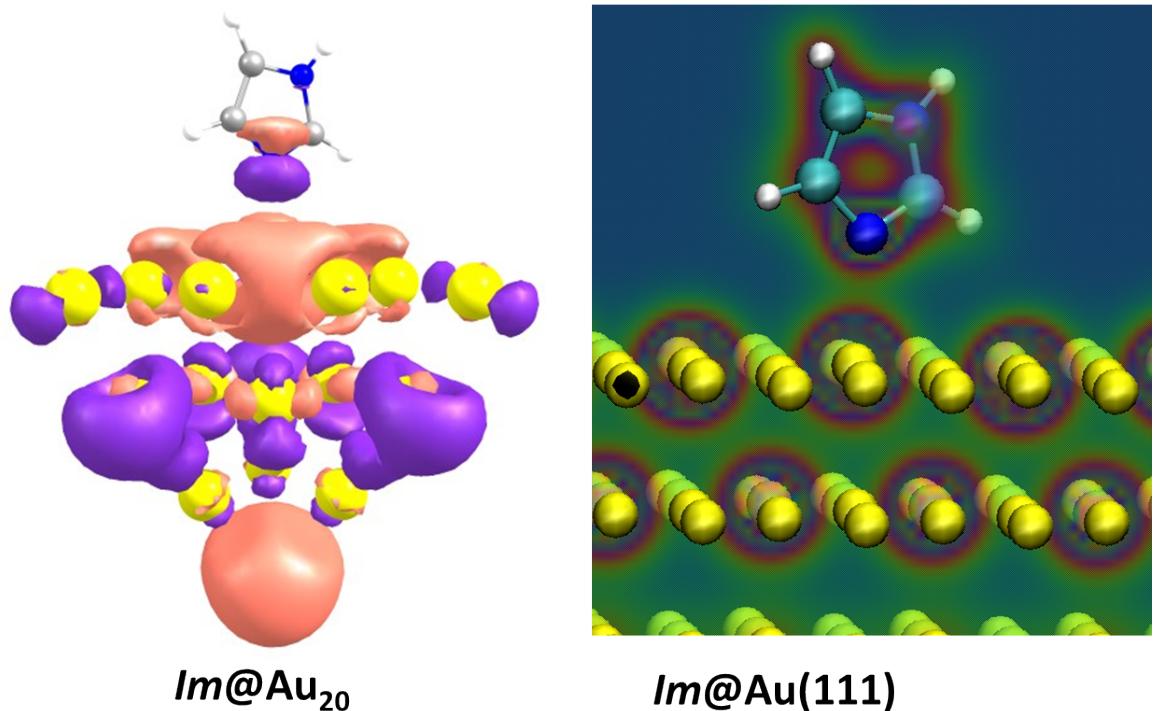


Figure S2: Iso surface and contour profile for CO₂-*Im* @Au₂₀ (iso surface value 0.02 a.u).

