Table S1. Adsorption energies (eV) for the different layers and freeze of atomic C on Pt(111) and Ni(111) surface.

Surfaces	E_{ads}	Surfaces	E_{ads}
Pt(111) 6 layers	7.47	Ni(111) 6 layers	6.92
Pt(111) 5 layers	7.41	Ni(111) 5 layers	6.89
Pt(111) 5 layers fixed 2 layer	7.41	Ni(111) 5 layers fixed 2 layer	6.91

Table S2. Convergence tests for various cutoff energies for the calculated lattice constant of nickel and platinum bulk.

	400 eV	500 eV	600 eV	exp value
Ni bulk	3.52 Å	3.52 Å	3.52 Å	3.51 Å
Pt bulk	3.99 Å	3.99 Å	3.99 Å	3.92 Å

Table S3. Convergence tests for various Monkhorst-Pack *k*-points for the calculated lattice constant of nickel and platinum bulk.

	3×3×3	4×4×4	5×5×5	6×6×6	7×7×7	8×8×8	9×9×9	10×10×10
Ni	3.51 Å	3.52 Å	3.52 Å	3.51 Å	3.52 Å	3.52 Å	3.52 Å	3.51 Å
Pt	3.98 Å	3.99 Å	3.99 Å	3.98 Å	3.99 Å	3.99 Å	3.99 Å	3.99 Å

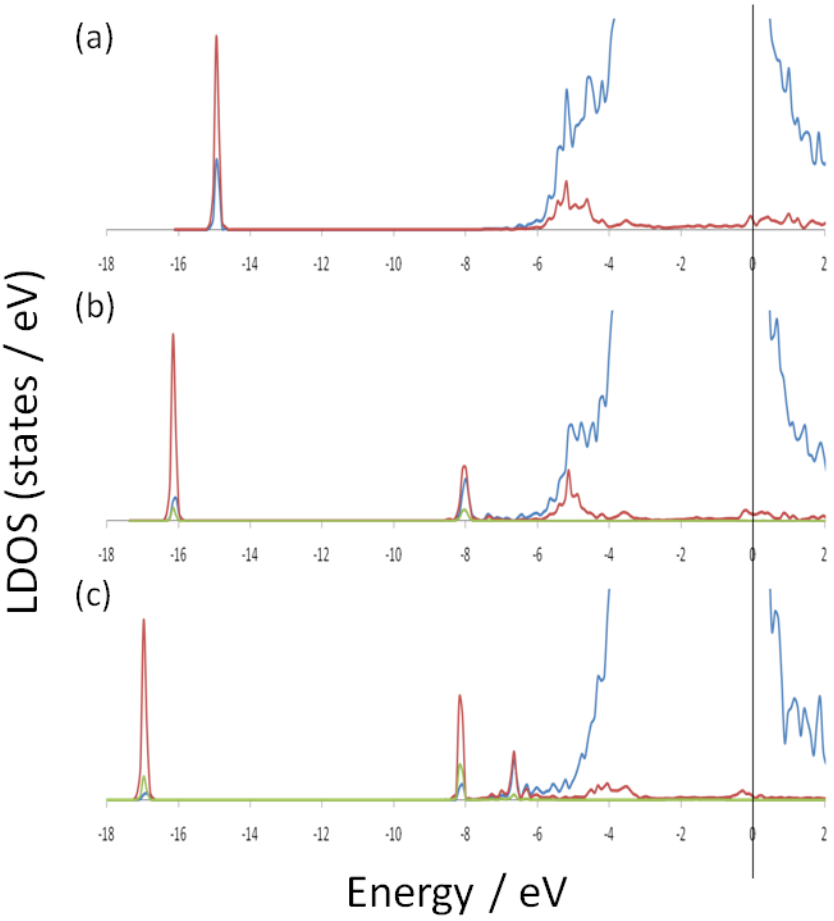

Figure S1. Local density of states (LDOS) for (a) N, (b) NH, and (c) NH_2 at fcc hollow site on Ni(111) surface. The blue, red and green lines represent d orbital of top layer Ni atoms, s and p orbital of N atom and H atom, respectively.

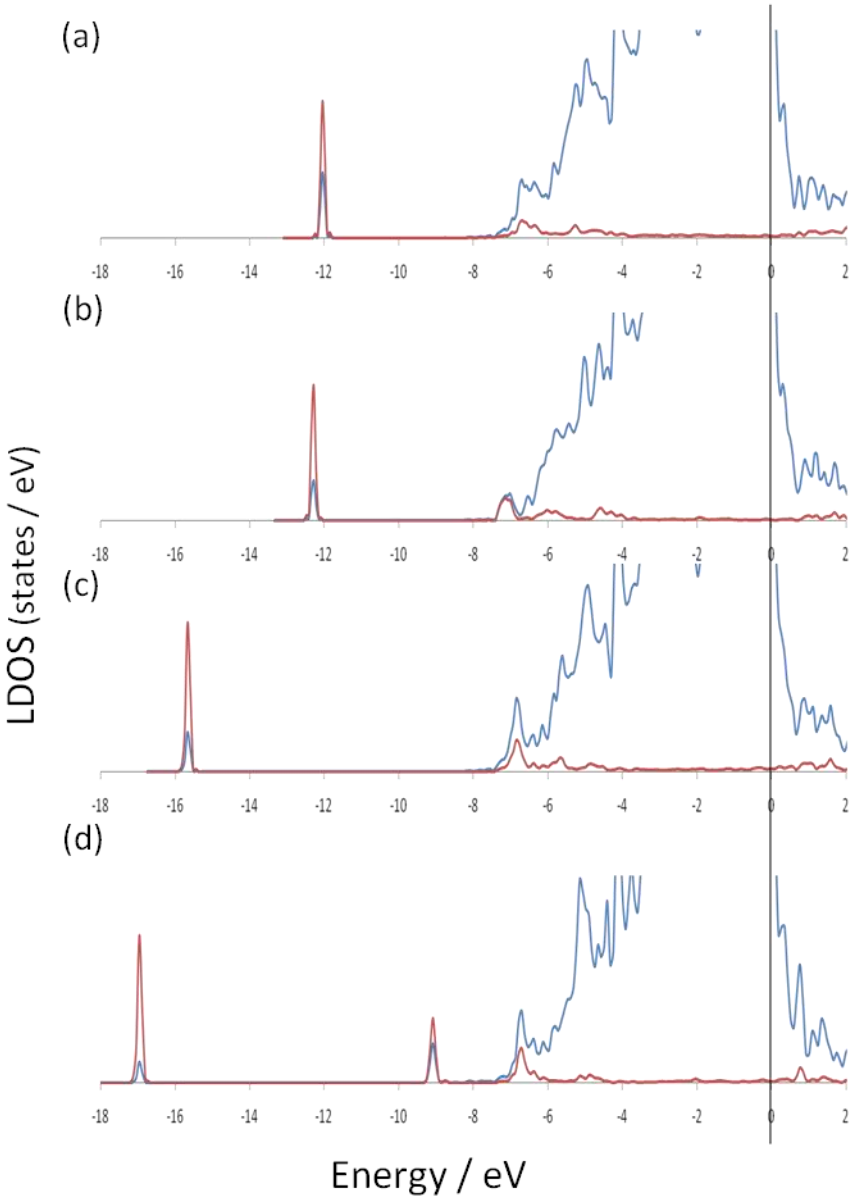

Figure S2. Local density of states (LDOS) for (a) C, (b) CH, (c) N, and (d) NH at fcc hollow site on Pt(111) surface. The blue and red lines represent d orbital of top layer Pt atoms and s and p orbital of C(N) atom, respectively.

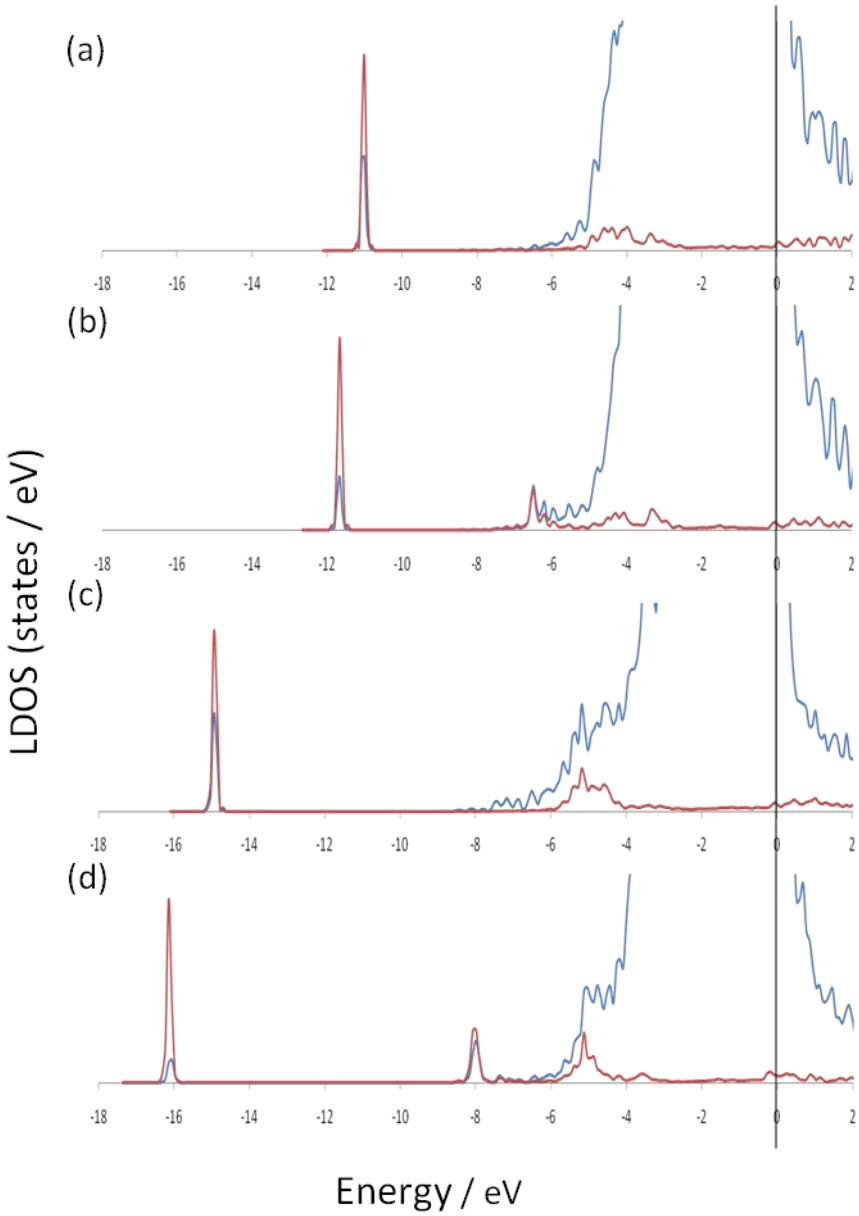

Figure S3. Local density of states (LDOS) for (a) C, (b) CH, (c) N, and (d) NH at fcc hollow site on Ni(111) surface. The blue and red lines represent d orbital of top layer Ni atoms and s and p orbital of C(N) atom, respectively.