Supplemental Information:

	Total Energy (eV)		
Strain	BDC	BDC+NH_2	BDC+NO_2
-0.0150	-161.5837	-170.8760	-197.8465
-0.0125	-161.5927	-170.8851	-197.8558
-0.0100	-161.6003	-170.8926	-197.8637
-0.0075	-161.6066	-170.8989	-197.8701
-0.0050	-161.6112	-170.9034	-197.8749
-0.0025	-161.6142	-170.9064	-197.8780
0.0000	-161.6152	-170.9073	-197.8790
0.0025	-161.6142	-170.9062	-197.8780
0.0050	-161.6109	-170.9028	-197.8746
0.0075	-161.6050	-170.8971	-197.8685
0.0100	-161.5965	-170.8884	-197.8597
0.0125	-161.5850	-170.8770	-197.8479
0.0150	-161.5702	-170.8623	-197.8326

Table 1: Total energy for thirteen strain calculation ranging from -1.5% to +1.5% for a PBE functional. Note, these energies reported are pseudopotential dependent.

	LUMO (eV)			HOMO (eV)		
Strain	BDC	BDC+NH_2	BDC+NO_2	BDC	BDC+NH_2	BDC+NO_2
-0.0150	1.360	1.850	1.730	-1.630	-0.110	-1.020
-0.0125	1.310	1.800	1.670	-1.670	-0.150	-1.060
-0.0100	1.260	1.740	1.620	-1.710	-0.190	-1.050
-0.0075	1.220	1.690	1.570	-1.750	-0.230	-1.150
-0.0050	1.170	1.640	1.510	-1.790	-0.270	-1.200
-0.0025	1.120	1.590	1.460	-1.830	-0.310	-1.230
0.0000	1.070	1.540	1.410	-1.870	-0.350	-1.270
0.0025	1.030	1.490	1.350	-1.910	-0.390	-1.310
0.0050	0.980	1.440	1.300	-1.950	-0.420	-1.350
0.0075	0.940	1.390	1.250	-1.980	-0.460	-1.390
0.0100	0.890	1.340	1.200	-2.020	-0.500	-1.430
0.0125	0.850	1.290	1.150	-2.060	-0.540	-1.470
0.0150	0.800	1.2519	1.100	-2.090	-0.570	-1.504

Table 2: The calculated LUMO and HOMO values for each of the designs. These were calculated using a PBE functional.