

Supporting Information

Nitrogen-Doped Borophene Quantum Dots: A Novel Sensing Material for Detection of Hazardous Environmental Gases

Kriengkri Timsorn ¹ and Chatchawal Wongchoosuk ^{2,*}

¹ Division of Physics, Faculty of Science and Technology, Phetchabun Rajabhat University, Phetchabun 67000, Thailand; timsorn23@pcru.ac.th

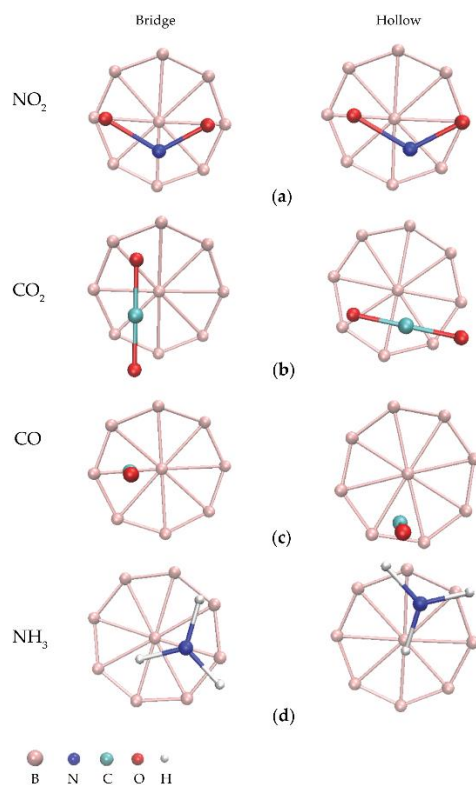
² Department of Physics, Faculty of Science, Kasetsart University, Chatuchak, Bangkok 10900, Thailand; chatchawal.w@ku.ac.th

* Correspondence: chatchawal.w@ku.ac.th; Tel.: +662-562-5555

Table S1: Typical calculated adsorption parameters for each gas molecule absorbed on the B₉⁻ BQD structures with bridge and hollow sites.

System	Adsorption sites	Distance (Å)	E _{ad} (eV)	Q (e)	E _{HOMO} (eV)	E _{LUMO} (eV)	E _g (eV)
B ₉ ⁻ - NO ₂	bridge	1.23	-5.66	-0.009	-6.11	-5.04	1.07
	hollow	1.23	-5.66	-0.009	-6.11	-5.04	1.07
B ₉ ⁻ - CO	bridge	1.12	-1.26	0.023	-5.89	-4.95	0.94
	hollow	1.12	-0.72	0.341	-5.63	-3.13	2.50
B ₉ ⁻ - CO ₂	bridge	1.75	-3.93	-0.027	-6.40	-4.61	1.79
	hollow	1.75	-3.05	-0.044	-5.70	-4.54	1.16
B ₉ ⁻ - NH ₃	bridge	3.00	-2.72	0.516	-4.81	-4.49	0.32
	hollow	3.00	-1.78	0.420	-5.14	-2.90	2.24

Figure S1: Some optimized B_9^- BQDs for adsorption of (a) NO_2 , (b) CO_2 , (c) CO and (d) NH_3 with bridge and hollow sites.



Source Code S1: An example of DFTB command code for full optimization.

```
Geometry = GenFormat {
<<< "1.23-A.gen"
}
Hamiltonian = DFTB {
  SCC = Yes
  SCCTolerance = 1e-6
  MaxSCCIterations = 1000
  Mixer = Broyden {}
  MaxAngularMomentum = {
    B = "p"
    N = "p"
    O = "p"
  }
  Charge = 0.0
  SpinPolarisation = {}
  Filling = Fermi {
    Temperature [K] = 300
```

```

}
Dispersion = LennardJones {
  Parameters {
    B {
      Distance [AA] = 4.083
      Energy [kcal/mol] = 0.180
    }
    N {
      Distance [AA] = 3.660
      Energy [kcal/mol] = 0.069
    }
    O {
      Distance [AA] = 3.500
      Energy [kcal/mol] = 0.060
    }
  }
}
SlaterKosterFiles = {
  B-B = "/opt/programs/DFTB+/TB-paras/matsci-0-3/B-B.skf"
  B-N = "/opt/programs/DFTB+/TB-paras/matsci-0-3/B-N.skf"
  B-O = "/opt/programs/DFTB+/TB-paras/matsci-0-3/B-O.skf"
  N-N = "/opt/programs/DFTB+/TB-paras/matsci-0-3/N-N.skf"
  N-O = "/opt/programs/DFTB+/TB-paras/matsci-0-3/N-O.skf"
  N-B = "/opt/programs/DFTB+/TB-paras/matsci-0-3/N-B.skf"
  O-O = "/opt/programs/DFTB+/TB-paras/matsci-0-3/O-O.skf"
  O-B = "/opt/programs/DFTB+/TB-paras/matsci-0-3/O-B.skf"
  O-N = "/opt/programs/DFTB+/TB-paras/matsci-0-3/O-N.skf"
}

KPointsAndWeights = SupercellFolding {
  1 0 0
  0 1 0
  0 0 1
  0.0 0.0 0.0
}
Driver = ConjugateGradient {
  LatticeOpt = Yes
  MovedAtoms = 1:-1
  MaxForceComponent = 1.0e-4
  MaxSteps = 10000
  OutputPrefix = "geo_end"
  Constraints = {}
}

```