|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **model** | **site** | **HOMO** | **LUMO** | **Eg eV** | **EF eV** |
|  | bridge | -6.693 | -4.163 | 1.061 | -0.463 |
| SO/O-doped BN | N | 5.197 | -5.197 | 1.061 | -0.001 |
|  | center | -7.537 | -3.999 | 3.538 | 0.001 |
|  | bridge | -6.176 | -5.061 | 3.565 | -0.006 |
| SO2/O-doped BN | N | -6.040 | -3.319 | 2.721 | 0 |
|  | center | -6.503 | -4.435 | 2.068 | 0.002 |
|  | bridge | -6.666 | -3.836 | 2.83  | 0.009 |
| NO/O-doped BN | N | -6.666 | -3.836 | 2.83  | -0.001 |
|  | center | -6.666 | -3.836 | 2.83  | 0.009 |
|  | bridge | -6.203 | -3.782 | 2.421 | -0.001 |
| NO2/O-dopedBN | N | -6.203 | -3.564 | 2.639 | 0.056 |
|  | center | -6.503 | -3.673 | 2.83 | 0 |
|  | bridge | -4.925 | -4.217 | 0.708eV | 0 |
| CO/O-dopedBN | N | -6.720 | -3.237 | 3.483 | 0.012 |
|  | center | -5.033 | -4.326 | 0.707eV | 0 |
|  | bridge | -6.530 | -4.816 | 1.714 | 0.002 |
| CO2/O-doped BN | N | -6.530 | -4.816 | 1.714 | 0.7 |
|  | center | -6.530 | -4.816 | 1.714 | 0.002 |
|  | bridge | -4.925 | -1.877 | 3.048 | 0.001 |
| NH3/O-doped BN | N | -4.380 | -2.149 | 2.231 | -0.001 |
|  | center | -5.850 | -3.673 | 2.177 | -0.047 |