**Electronic Supporting Information**

Adsorption of the guanine molecule over the pristine, Nb- and Au-doped boron nitride nanosheets: a DFT study

Meryem Derdare, Abdel-Ghani Boudjahem \*

Computational Catalysis Group, Laboratory of Applied Chemistry, University of Guelma, Box 401, 24000, Guelma, Algeria

\* Author corresponding

E-mail address: [Boudjahem@yahoo.fr](mailto:Boudjahem@yahoo.fr) (A. Boudjahem)

Figure S1. The most stable complexes obtained upon interaction of the guanine molecule with the surface of the NbBN cluster (H, I, J, K and L).

|  |  |
| --- | --- |
| (H) | |
| (I) | (J) |
| (K) | (L) |

Figure S2. Frontier molecular orbitals (FMO) plots of the Nb-doped BN nanosheet and their formed complexes upon interaction with the guanine molecule (H, I, J, K and L).

|  |  |
| --- | --- |
| HOMO LUMO | |
|  |  |
| Au-BN | |
|  |  |
| Complex C | |
|  |  |
| Complex D | |
|  |  |
| Complex E | |
|  |  |
| Complex F | |
|  |  |
| Complex G | |

Figure S3. The electron density difference (EDD) isosurfaces for the complexes H, I, J, K and L.

|  |  |  |  |
| --- | --- | --- | --- |
|  | (H) | |  |
| (I) | | (J) | |
| (K) | | (L) | |