Supporting Information

Understanding of Light Absorption Properties of the N-Doped Graphene Oxide Quantum Dot with TD-DFT

Mohammed A. Jabed[1], Julia Zhao[1], Dmitri Kilin[2], Tao Yu[1*]

[1.] *Department of Chemistry, University of North Dakota, Grand Forks, ND 58202*
[2.] *Department of Chemistry, North Dakota State University, Fargo, ND 58105*

Calculation of the Distortion plot:

We employed two analysis tools to investigate the structure feature and charge transfer character of the considered systems. In particular, we noticed that both edge modification and N-doping could distort the graphene planar structure. The distortion from the planar graphene structures are characterized by the perpendicular distance of each coordinate from a plane (p), where the plane p is defined by three coordinate $(\boldsymbol{r}_a, \boldsymbol{r}_b, \boldsymbol{r}_c)$ and the distance is -

$$d = \frac{\boldsymbol{n}_p * \boldsymbol{r}_i}{|\boldsymbol{n}|} \ ; i = 1, 2, 3 \dots \dots N \tag{S1}$$

$\boldsymbol{n}_p$ is the norm vector of the plane $\boldsymbol{P}(\boldsymbol{r}_a, \boldsymbol{r}_b, \boldsymbol{r}_c)$, and N is the total number of atoms. The three coordinate vectors $(\boldsymbol{r}_a, \boldsymbol{r}_b, \boldsymbol{r}_c)$ of the plane, P is defined as –

$$\sum_{i=1}^{N} \boldsymbol{d}^2_{(r_a,r_b,r_c),r_i} \leq \sum_{i=1}^{N} \boldsymbol{d}^2_{(r_l,r_m,r_n),r_i} \quad where \ l, m, n \in N \tag{S2}$$

The positive and negative distances indicate the upward and downward distortion from the reference plane, which is comparable with the pristine graphene's planer conformation.
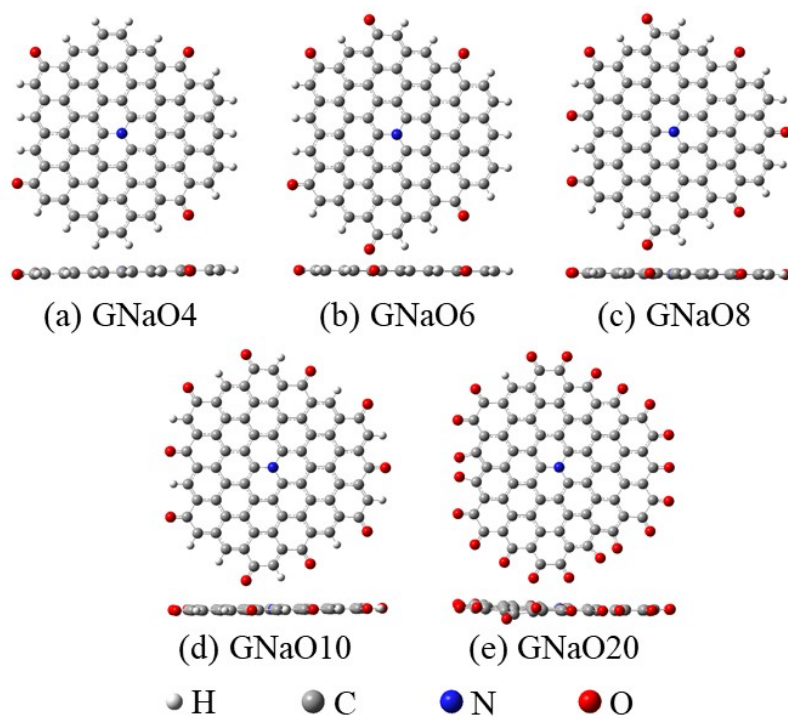
Figure S1: The top and side view of the optimized N-doped graphene oxides quantum dots with a different number of =O groups on edge. The optimized geometries using the PBE0/6-31G* method.
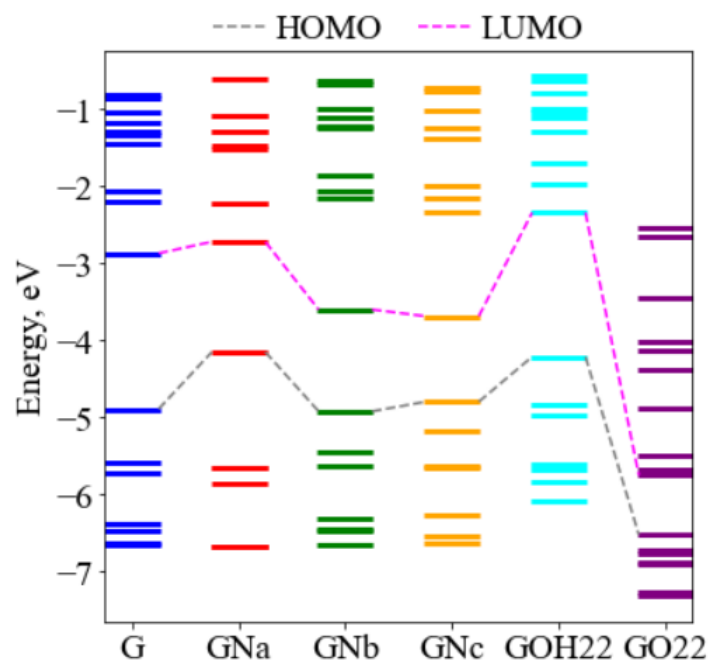
Figure S2: The molecular orbital energy diagrams of the quantum dots of pristine graphene, N-doped graphene, graphene with edge oxidation. Dotted connected lines indicate the highest occupied (gray) and the lowest unoccupied (magenta) molecular orbitals energy.
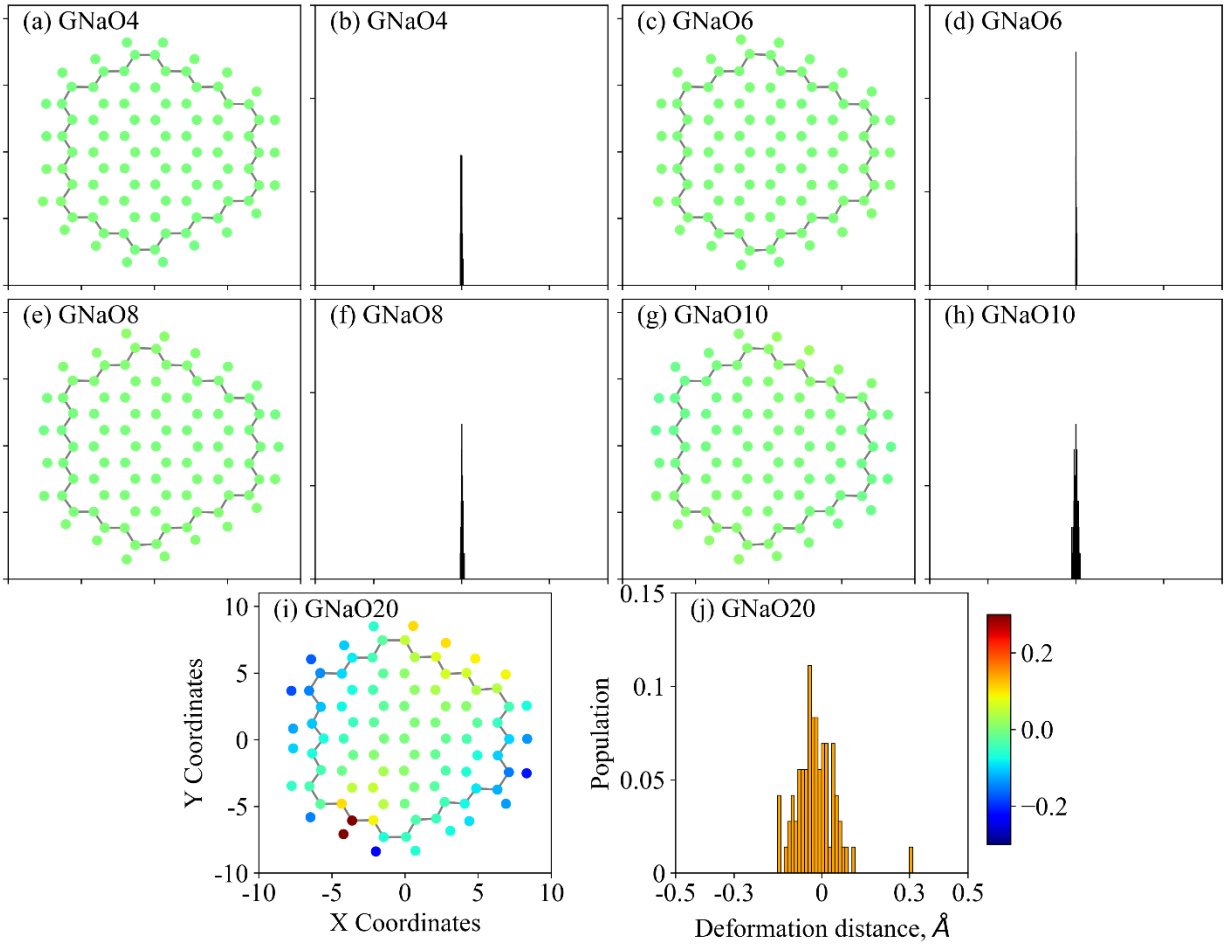
Figure S3: The deformation maps (a, c, e, g, i) and its normalized histogram distribution (b, d, f, h, j) of the GNaO4, GNaO6, GNaO8, GNaO10, and GNaO20 quantum dots, respectively. Color coding indicates the deformation distance calculated by the equation S1. The gray line indicates the edge carbons of the graphene QDs.
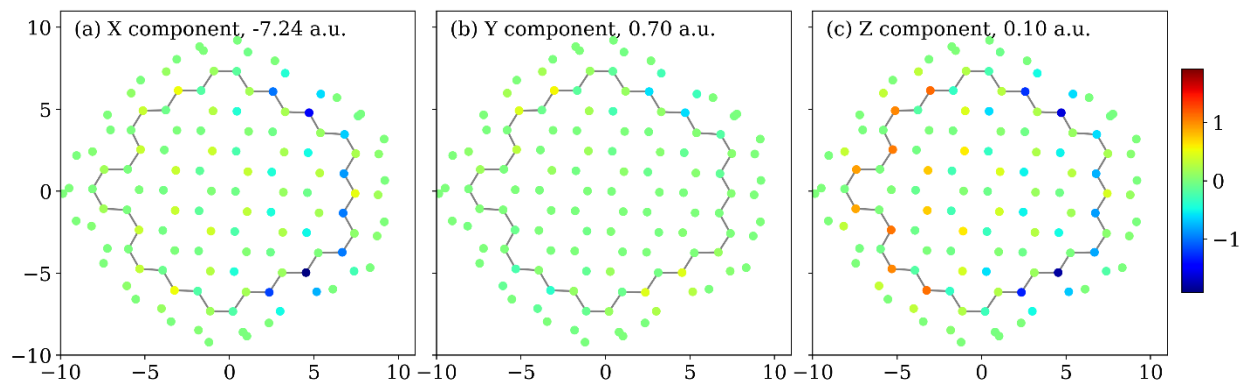
Figure S4: The maps of the X-, Y-, Z-component of the atomic transition dipole moment of the S_1 states for GOH22. The magnitude is the decomposition of the molecular transition dipole moment on each atom. The gray line indicates the edge carbons of the quantum dot.
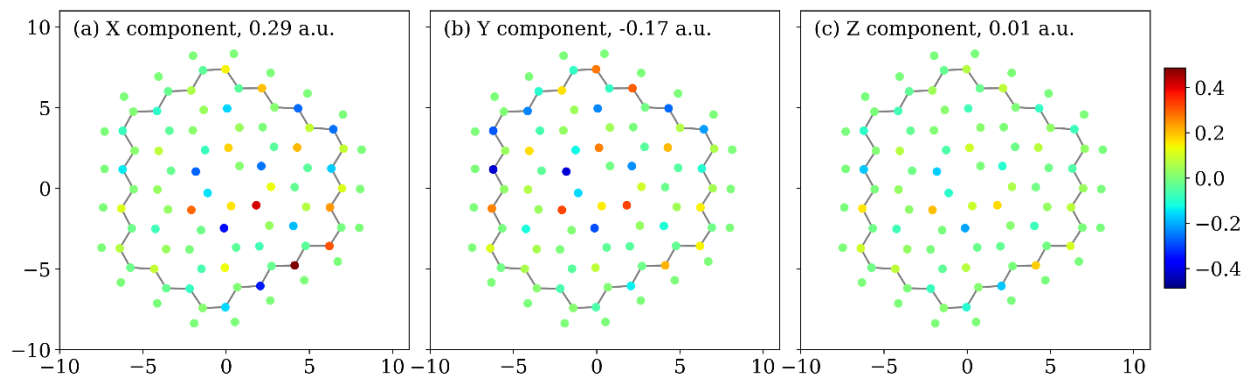
Figure S5: The maps of the X-, Y-, Z-component of the atomic transition dipole moment of the S_1 states for GNb. The magnitude is the decomposition of the molecular transition dipole moment on each atom. The gray line indicates the edge carbons of the quantum dot.
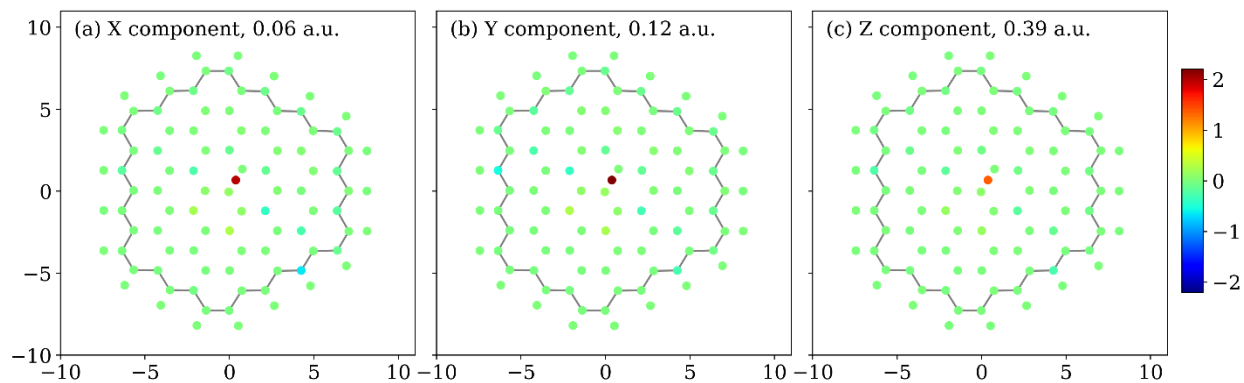
Figure S6: The maps of the X-, Y-, Z-component of the atomic transition dipole moment of the S_1 states for GNc. The magnitude is the decomposition of the molecular transition dipole moment on each atom. The gray line indicates the edge carbons of the quantum dot.
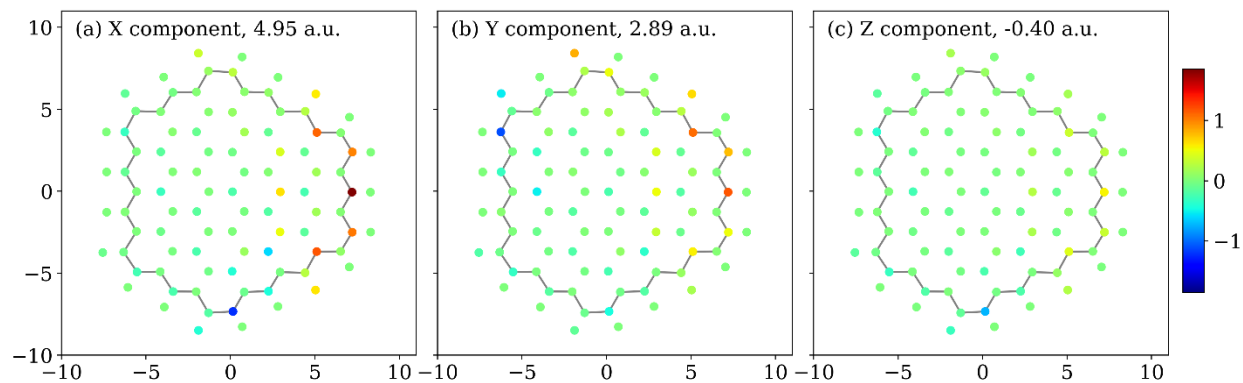
Figure S7: The maps of the X-, Y-, Z-component of the atomic transition dipole moment of the S_1 states for GNaO6. The magnitude is the decomposition of the molecular transition dipole moment on each atom. The gray line indicates the edge carbons of the quantum dot.
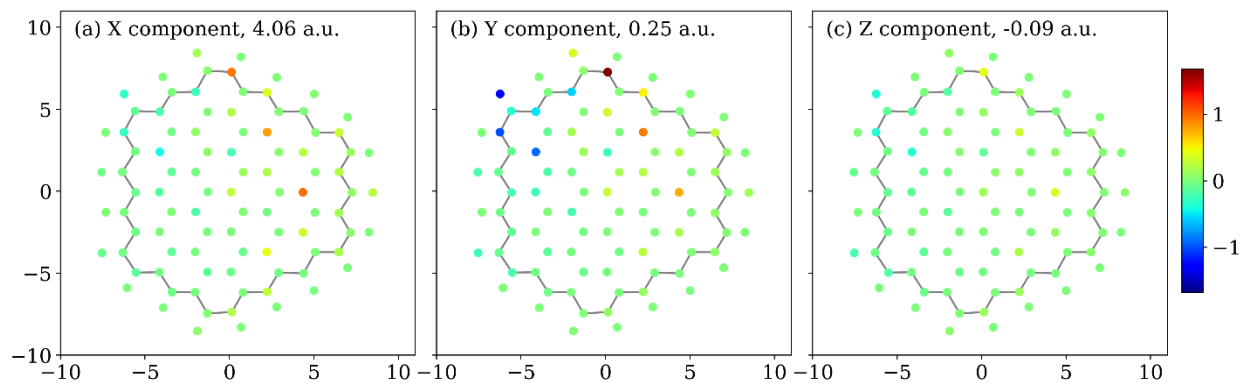
Figure S8: The maps of the X-, Y-, Z-component of the atomic transition dipole moment of the S_1 states for GNaO8. The magnitude is the decomposition of the molecular transition dipole moment on each atom. The gray line indicates the edge carbons of the quantum dot.
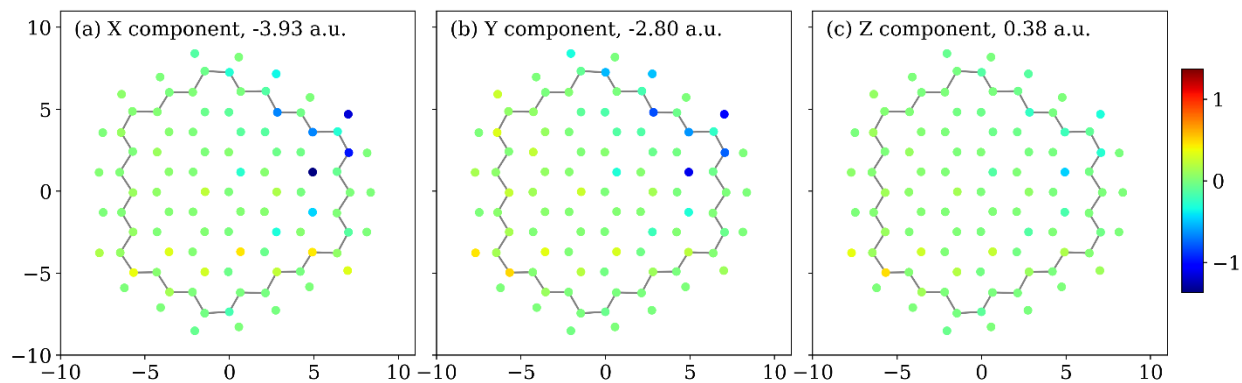
Figure S9: The maps of the X-, Y-, Z-component of the atomic transition dipole moment of the S_1 states for GNaO10. The magnitude is the decomposition of the molecular transition dipole moment on each atom. The gray line indicates the edge carbons of the quantum dot.