Supplementary Information

The Fluorescent Quenching Mechanism of N and S Co-Doped Graphene Quantum Dots with Fe$^{3+}$ and Hg$^{2+}$ Ions and Their Application as a Novel Fluorescent Sensor

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Table 1. The atomic populations of Fe$^{3+}$@N, S-GQDs and Hg$^{2+}$@N,S-GQDs.

| Materials | s   | p   | d   | Total | Charge (e) | Bond Population | d (Å) |
|-----------|-----|-----|-----|-------|------------|-----------------|-------|
| Fe$^{3+}$ | C4  | 1.20| 2.98| 4.18  | -0.18      | C1-O            | 0.48  | 1.43 |
|           | C9  | 1.09| 3.02| 4.12  | -0.12      | C1-S            | 0.53  | 1.76 |
|           | C10 | 1.26| 2.92| 4.18  | -0.18      | C2-S            | 0.64  | 1.70 |
|           | N   | 1.40| 3.84| 5.23  | -0.24      | C2-N            | 0.88  | 1.39 |
|           | O   | 1.81| 4.60| 6.42  | -0.42      | C3-N            | 0.83  | 141  |
|           | S   | 1.63| 3.60| 5.22  | 0.78       | C3-O            | -0.05 | 2.63 |
|           | Fe  | 0.28| -0.10|7.16  | 7.34       | 0.66            | Fe-O  | 2.64 |
|           |     |     |     |       |            | Fe-S            | 0.17  | 2.03 |
|           |     |     |     |       |            | Fe-N            | -0.17 | 2.80 |
| Hg$^{2+}$ | C4  | 1.36| 2.83| 4.19  | -0.19      | C1-O            | 0.32  | 1.57 |
|           | C9  | 1.07| 3.07| 4.14  | -0.14      | C1-S            | 0.43  | 1.76 |
|           | C10 | 1.03| 2.75| 3.77  | 0.23       | C2-S            | 0.59  | 1.71 |
|           | N   | 1.39| 3.87| 5.25  | -0.25      | C2-N            | 0.86  | 1.39 |
|           | O   | 1.73| 4.55| 6.28  | -0.28      | C3-N            | 0.91  | 1.41 |
|           | S   | 1.70| 3.50| 5.20  | 0.80       | C3-O            | 0.50  | 1.51 |
|           | Hg  | 1.87| 0.01|10.0   | 11.87      | 0.13            | Hg-O  | -0.07| 3.37 |
|           |     |     |     |       |            | Hg-S            | -0.06 | 3.85 |
|           |     |     |     |       |            | Hg-N            | -0.13 | 3.24 |
Table S2 Recovery of Fe$^{3+}$ and Hg$^{2+}$ detection in drinking water samples.

| Sample                      | Spiked concentration | Detected concentration | Recovery ± RSD (%) |
|-----------------------------|----------------------|-------------------------|--------------------|
| Fe$^{3+}$ in Drinking water | 700 nM               | 654 nM                  | 93 ± 4.1           |
|                             | 1 μM                 | 1.27 μM                 | 127 ± 5.3          |
|                             | 3 μM                 | 3.63 μM                 | 121 ± 6.6          |
| Hg$^{2+}$ in Drinking water | 50 nM                | 62 nM                   | 124 ± 3.4          |
|                             | 100 nM               | 114 nM                  | 114 ± 4.6          |
|                             | 300 nM               | 284 nM                  | 95 ± 7.6           |
Figure S1. The schematic diagram of detection device geometry and testing process.
Figure S2. The stability of fluorescence intensity of as-synthesized N, S-GQDs solutions.
Figure S3. The fluorescence intensity of N, S-GQDs in real sample detection.