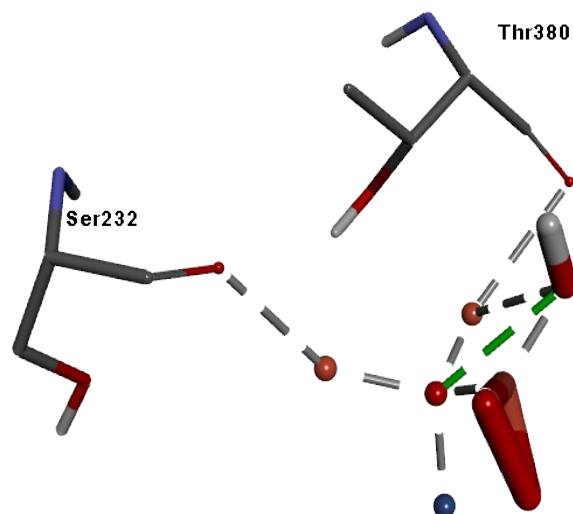
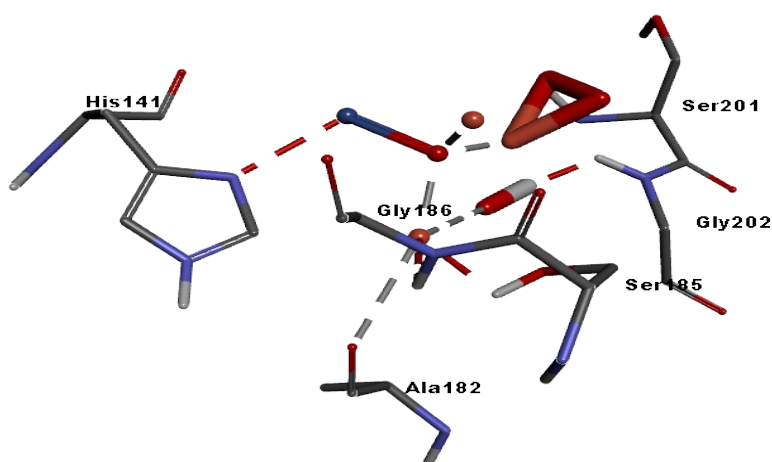


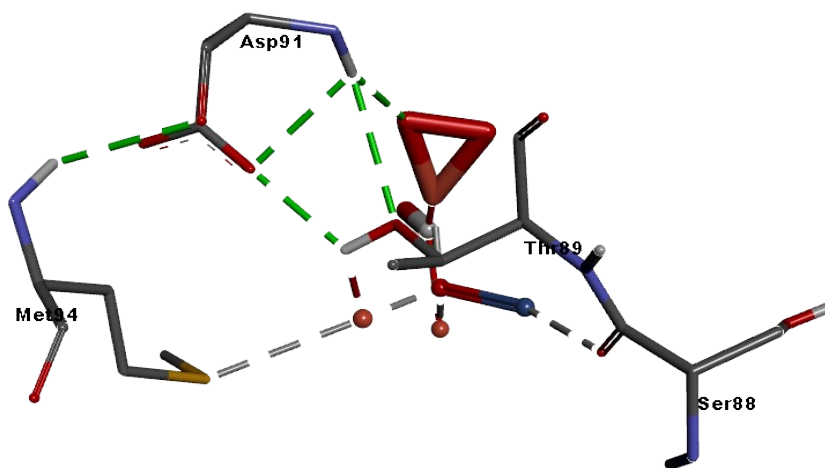
### Supplementary Information



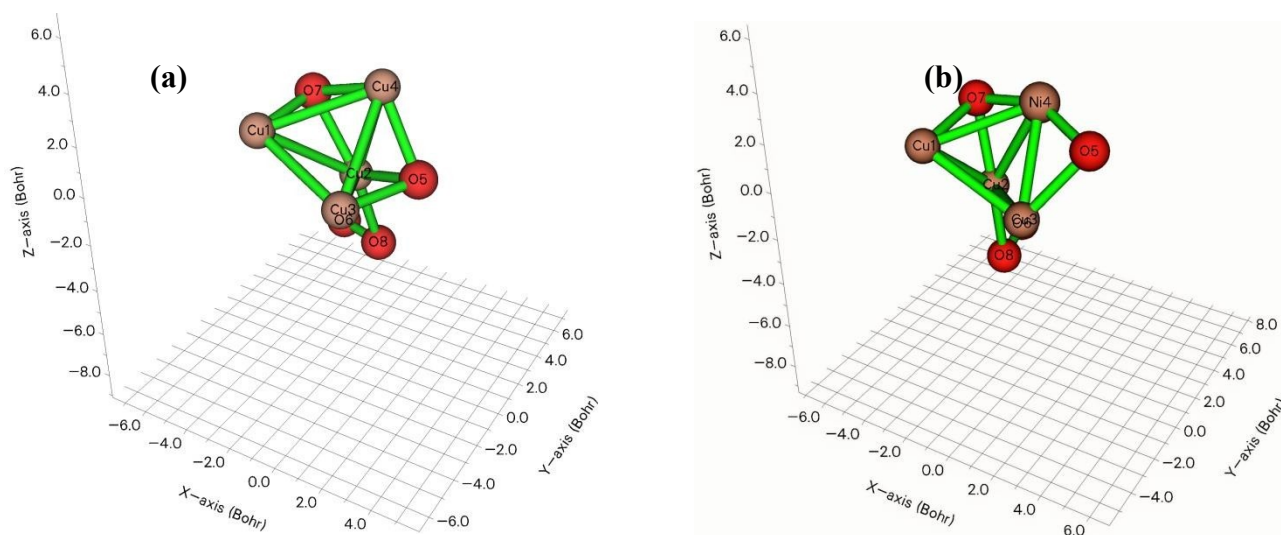
**Fig. S1** Non-bonding interactions of  $\text{Cu}_3\text{NiO}_4$  nanocluster against (a) 6AKZ (pose predicted by AutoDock Vina)



**Fig. S2** Non-bonding interactions of  $\text{Cu}_3\text{NiO}_4$  nanocluster against (a) 3ZMI (pose predicted by AutoDock Vina)



**Fig. S3** Non-bonding interactions of  $\text{Cu}_3\text{NiO}_4$  nanocluster against (a) 6IAI (pose predicted by AutoDock Vina)



**Fig. S4** 3D image of optimized nanocluster (a)  $\text{Cu}_4\text{O}_4$  and (b)  $\text{Cu}_3\text{NiO}_4$  visualized by Multiwfn.

**Table. S1** Raw OD data and statistical markers (RSD, p-values) of Ni-doped CuO and Pure CuO Nanoparticles

| Microorganism    | Cons(ppm) | Pure CuO<br>(Mean $\pm$ SD) | Ni-CuO<br>(Mean $\pm$ SD) | p-value | Pure CuO<br>Inhibition (%) $\pm$ SD | Ni-CuO Inhibition<br>(%) $\pm$ SD |
|------------------|-----------|-----------------------------|---------------------------|---------|-------------------------------------|-----------------------------------|
| <i>B. cereus</i> | 0         | 1.348 $\pm$ 0.155           | 1.348 $\pm$ .155          | 1       | 0 $\pm$ 0                           | 0 $\pm$ 0                         |
| <i>B. cereus</i> | 50        | 0.266 $\pm$ 0.001           | 0.239 $\pm$ .001          | 0.0001  | 80.27 $\pm$ 2.27                    | 82.26 $\pm$ 2.04                  |

|                  |     |               |              |        |              |              |
|------------------|-----|---------------|--------------|--------|--------------|--------------|
| <i>B. cereus</i> | 100 | 0.192 ± 0.002 | 0.183 ± .000 | 0.0003 | 85.76 ± 1.64 | 86.42 ± 1.56 |
| <i>B. cereus</i> | 150 | 0.160 ± 0.001 | 0.148 ± .001 | 0.0002 | 88.13 ± 1.37 | 89.02 ± 1.26 |
| <i>B. cereus</i> | 200 | 0.125 ± 0.001 | 0.136 ± .001 | 0.0001 | 90.73 ± 1.07 | 89.91 ± 1.16 |
| <i>B. cereus</i> | 250 | 0.112 ± 0.000 | 0.051 ± .001 | 0.0001 | 91.69 ± 0.96 | 96.22 ± 0.44 |
| <i>E. coli</i>   | 0   | 1.348 ± 0.167 | 1.348 ± .167 | 1      | 0 ± 0        | 0 ± 0        |
| <i>E. coli</i>   | 50  | 0.527 ± 0.001 | 0.361 ± .003 | 0.0001 | 60.89 ± 2.11 | 73.23 ± 1.98 |
| <i>E. coli</i>   | 100 | 0.448 ± 0.001 | 0.341 ± .002 | 0.0002 | 66.75 ± 1.88 | 74.71 ± 1.63 |
| <i>E. coli</i>   | 150 | 0.369 ± 0.001 | 0.309 ± .001 | 0.0003 | 72.62 ± 1.47 | 77.08 ± 1.42 |
| <i>E. coli</i>   | 200 | 0.360 ± 0.001 | 0.280 ± .001 | 0.0001 | 73.30 ± 1.36 | 79.22 ± 1.29 |
| <i>E. coli</i>   | 250 | 0.260 ± 0.001 | 0.180 ± .001 | 0.0001 | 80.70 ± 1.12 | 86.65 ± 0.96 |
| <i>S. aureus</i> | 0   | 1.448 ± 0.058 | 1.448 ± .058 | 1      | 0 ± 0        | 0 ± 0        |
| <i>S. aureus</i> | 50  | 0.269 ± 0.001 | 0.363 ± .005 | 0.0002 | 81.42 ± 2.07 | 74.93 ± 2.44 |
| <i>S. aureus</i> | 100 | 0.136 ± 0.001 | 0.152 ± .002 | 0.0003 | 90.61 ± 1.33 | 89.50 ± 1.47 |
| <i>S. aureus</i> | 150 | 0.123 ± 0.000 | 0.142 ± .000 | 0.0001 | 91.51 ± 1.21 | 90.19 ± 1.33 |
| <i>S. aureus</i> | 200 | 0.109 ± 0.002 | 0.103 ± .001 | 0.045  | 92.47 ± 0.94 | 92.89 ± 1.11 |
| <i>S. aureus</i> | 250 | 0.085 ± 0.001 | 0.090 ± .004 | 0.06   | 94.13 ± 0.88 | 93.78 ± 0.92 |
| <i>S. typhi</i>  | 0   | 1.095 ± 0.004 | 1.095 ± .004 | 1      | 0 ± 0        | 0 ± 0        |
| <i>S. typhi</i>  | 50  | 0.443 ± 0.001 | 0.436 ± .001 | 0.018  | 59.54 ± 1.83 | 60.18 ± 1.76 |
| <i>S. typhi</i>  | 100 | 0.376 ± 0.002 | 0.280 ± .000 | 0.0001 | 65.71 ± 1.55 | 74.20 ± 1.42 |
| <i>S. typhi</i>  | 150 | 0.328 ± 0.001 | 0.244 ± .004 | 0.0001 | 70.04 ± 1.37 | 77.72 ± 1.19 |
| <i>S. typhi</i>  | 200 | 0.320 ± 0.001 | 0.241 ± .001 | 0.0001 | 70.77 ± 1.26 | 77.99 ± 1.13 |
| <i>S. typhi</i>  | 250 | 0.254 ± 0.001 | 0.235 ± .001 | 0.005  | 76.82 ± 1.03 | 78.54 ± 1.02 |
| <i>Candida</i>   | 0   | 1.410 ± 0.054 | 1.410 ± .054 | 1      | 0 ± 0        | 0 ± 0        |
| <i>Candida</i>   | 50  | 0.459 ± 0.001 | 0.336 ± .001 | 0.0001 | 67.45 ± 2.36 | 76.17 ± 2.17 |
| <i>Candida</i>   | 100 | 0.047 ± 0.002 | 0.203 ± .027 | 0.0001 | 96.67 ± 0.91 | 85.60 ± 2.01 |
| <i>Candida</i>   | 150 | 0.044 ± 0.001 | 0.040 ± .001 | 0.12   | 96.88 ± 0.88 | 97.16 ± 0.86 |
| <i>Candida</i>   | 200 | 0.030 ± 0.000 | 0.037 ± .000 | 0.001  | 97.87 ± 0.65 | 97.37 ± 0.74 |
| <i>Candida</i>   | 250 | 0.022 ± 0.002 | 0.004 ± .001 | 0.0001 | 98.44 ± 0.57 | 99.72 ± 0.31 |

**Table. S2** For pure Cu<sub>4</sub>O<sub>4</sub>

Atom list:

1(Cu) --> Charge: 29.000000 x,y,z(Bohr): -3.646776 -1.698589 1.451011

2(Cu) --> Charge: 29.000000 x,y,z(Bohr): -1.520289 1.832990 -1.465825

3(Cu) --> Charge: 29.000000 x,y,z(Bohr): 0.460557 -2.735949 -0.121893

4(Cu) --> Charge: 29.000000 x,y,z(Bohr): -0.036005 1.125721 2.896028  
 5(O ) --> Charge: 8.000000 x,y,z(Bohr): 1.870667 0.459827 -0.090624  
 6(O ) --> Charge: 8.000000 x,y,z(Bohr): -3.148294 3.646611 -5.104466  
 7(O ) --> Charge: 8.000000 x,y,z(Bohr): -3.417271 1.796183 1.673463  
 8(O ) --> Charge: 8.000000 x,y,z(Bohr): -0.920745 2.661002 -4.940697

Range of alpha orbitals: 1 - 180 Range of beta orbitals: 181 - 360

Note: Orbital 75 is alpha-HOMO, energy: -0.170443 a.u. -4.638000 eV

Orbital 253 is beta-HOMO, energy: -0.177136 a.u. -4.820114 eV

Orbital 76 is alpha-LUMO, energy: -0.159309 a.u. -4.335020 eV

Orbital 254 is beta-LUMO, energy: -0.152447 a.u. -4.148300 eV

HOMO-LUMO gap of alpha orbitals: 0.011134 a.u. 0.302980 eV

HOMO-LUMO gap of beta orbitals: 0.024689 a.u. 0.671814 eV

### Ni doped

Atom list:

1(Cu) --> Charge: 29.000000 x,y,z(Bohr): -3.349883 -1.775015 1.210816  
 2(Cu) --> Charge: 29.000000 x,y,z(Bohr): -2.415477 1.533645 -1.799938  
 3(Cu) --> Charge: 29.000000 x,y,z(Bohr): 0.889447 -1.774252 -0.694176  
 4(Ni) --> Charge: 28.000000 x,y,z(Bohr): -0.079775 1.222912 2.529244  
 5(O ) --> Charge: 8.000000 x,y,z(Bohr): 2.777131 -0.202340 1.889388  
 6(O ) --> Charge: 8.000000 x,y,z(Bohr): -2.695507 4.296570 -5.194900  
 7(O ) --> Charge: 8.000000 x,y,z(Bohr): -3.316878 1.888530 1.689866  
 8(O ) --> Charge: 8.000000 x,y,z(Bohr): -2.167215 1.897745 -5.333303

Range of alpha orbitals: 1 - 180 Range of beta orbitals: 181 - 360

Note: Orbital 74 is alpha-HOMO, energy: -0.184311 a.u. -5.015357 eV

Orbital 253 is beta-HOMO, energy: -0.182998 a.u. -4.979623 eV

Orbital 75 is alpha-LUMO, energy: -0.157844 a.u. -4.295167 eV

Orbital 254 is beta-LUMO, energy: -0.156003 a.u. -4.245047 eV

HOMO-LUMO gap of alpha orbitals: 0.026466 a.u. 0.720190 eV

**Table. S3** Mulliken charge for pure

| Atom  | Alpha pop. | Beta pop. | Spin pop. | Atomic charge |
|-------|------------|-----------|-----------|---------------|
| 1(Cu) | 14.37921   | 14.41973  | -0.04052  | 0.20107       |

|       |          |          |          |          |
|-------|----------|----------|----------|----------|
| 2(Cu) | 14.37254 | 14.18319 | 0.18934  | 0.44427  |
| 3(Cu) | 14.55969 | 14.27048 | 0.28922  | 0.16983  |
| 4(Cu) | 14.32041 | 14.34288 | -0.02247 | 0.33671  |
| 5(O ) | 4.39373  | 4.06083  | 0.3329   | -0.45456 |
| 6(O ) | 4.43513  | 3.65295  | 0.78218  | -0.08808 |
| 7(O ) | 4.15264  | 4.32254  | -0.16991 | -0.47518 |
| 8(O ) | 4.38666  | 3.7474   | 0.63925  | -0.13406 |

Total net charge: -0.00000000 Total spin electrons: 2.00000000

**Table. S4** Mulliken charge for dope

| Atom  | Alpha pop. | Beta pop. | Spin pop. | Atom  |
|-------|------------|-----------|-----------|-------|
| 1(Cu) | 14.45887   | 14.31873  | 0.14014   | 1(Cu) |
| 2(Cu) | 14.30662   | 14.37139  | -0.06478  | 2(Cu) |
| 3(Cu) | 14.48461   | 14.27622  | 0.20839   | 3(Cu) |
| 4(Ni) | 14.36991   | 13.20843  | 1.16148   | 4(Ni) |
| 5(O ) | 4.51666    | 3.93725   | 0.5794    | 5(O ) |
| 6(O ) | 3.68399    | 4.41693   | -0.73293  | 6(O ) |
| 7(O ) | 4.37987    | 4.11137   | 0.2685    | 7(O ) |
| 8(O ) | 3.79948    | 4.35969   | -0.56021  | 8(O ) |

Total net charge: -0.00000000 Total spin electrons: 1.00000000

**Table. S5** Lowdin charge for pure

| Atom  | Alpha pop. | Beta pop. | Spin pop. | Atomic charge |
|-------|------------|-----------|-----------|---------------|
| 1(Cu) | 14.39514   | 14.44111  | -0.04597  | 0.16374       |
| 2(Cu) | 14.47817   | 14.27391  | 0.20426   | 0.24793       |
| 3(Cu) | 14.57354   | 14.28683  | 0.28671   | 0.13962       |
| 4(Cu) | 14.37743   | 14.39398  | -0.01655  | 0.22858       |
| 5(O ) | 4.32246    | 4.00256   | 0.3199    | -0.32503      |
| 6(O ) | 4.43201    | 3.65377   | 0.77824   | -0.08578      |
| 7(O ) | 4.08225    | 4.24567   | -0.16342  | -0.32792      |
| 8(O ) | 4.33899    | 3.70215   | 0.63684   | -0.04114      |

Total net charge: -0.00000000 Total spin electrons: 2.00000000

**Table. S6** Lowdin charge for dope

| Atom  | Alpha pop. | Beta pop. | Spin pop. | Atomic charge |
|-------|------------|-----------|-----------|---------------|
| 1(Cu) | 14.46643   | 14.32529  | 0.14114   | 0.20828       |

|       |          |          |          |          |
|-------|----------|----------|----------|----------|
| 2(Cu) | 14.38429 | 14.44315 | -0.05886 | 0.17256  |
| 3(Cu) | 14.50444 | 14.30515 | 0.19929  | 0.1904   |
| 4(Ni) | 14.46557 | 13.30289 | 1.16268  | 0.23153  |
| 5(O ) | 4.44261  | 3.86836  | 0.57425  | -0.31098 |
| 6(O ) | 3.68731  | 4.41398  | -0.72668 | -0.10129 |
| 7(O ) | 4.29775  | 4.03064  | 0.26711  | -0.32838 |
| 8(O ) | 3.75159  | 4.31053  | -0.55893 | -0.06212 |

Total net charge: -0.00000000    Total spin electrons: 1.00000000

**Table. S7** Bond length for both systems

| Atom 1 | Atom 2 (Central) | Bond Length (Å) | System                                 |
|--------|------------------|-----------------|----------------------------------------|
| Cu1    | O7               | 1.884           | Pure Cu <sub>4</sub> O <sub>4</sub>    |
| Cu4    | O5               | 1.949           | Pure Cu <sub>4</sub> O <sub>4</sub>    |
| Cu4    | Cu3              | 2.321           | Pure Cu <sub>4</sub> O <sub>4</sub>    |
| Ni4    | O5               | 1.723           | Doped Cu <sub>3</sub> NiO <sub>4</sub> |
| Ni4    | O7               | 1.8             | Doped Cu <sub>3</sub> NiO <sub>4</sub> |
| Cu3    | O5               | 1.947           | Doped Cu <sub>3</sub> NiO <sub>4</sub> |
| Cu2    | O6               | 1.857           | Doped Cu <sub>3</sub> NiO <sub>4</sub> |
| Cu2    | O8               | 1.862           | Doped Cu <sub>3</sub> NiO <sub>4</sub> |

**Table. S8** Bond angle for both systems

| Atom 1 | Central Atom | Atom 3 | Bond Angle (°) | System                                 |
|--------|--------------|--------|----------------|----------------------------------------|
| O7     | Cu1          | Cu3    | 101.02         | Pure Cu <sub>4</sub> O <sub>4</sub>    |
| Cu2    | O6           | O8     | 55.8           | Pure Cu <sub>4</sub> O <sub>4</sub>    |
| Cu3    | O5           | Cu4    | 87.87          | Pure Cu <sub>4</sub> O <sub>4</sub>    |
| O7     | Ni4          | O5     | 150.46         | Doped Cu <sub>3</sub> NiO <sub>4</sub> |
| Cu2    | O6           | O8     | 54.24          | Doped Cu <sub>3</sub> NiO <sub>4</sub> |
| Cu3    | O5           | Ni4    | 82.58          | Doped Cu <sub>3</sub> NiO <sub>4</sub> |

**Table. S9** Photocatalytic and antibacterial performance comparison of undoped CuO, Ni–CuO (this work), and other doped CuO systems.

| Material / System    | Pollutant / Microorganism | Photocatalytic degradation (%) / Time | Rate constant <i>k</i> (min <sup>-1</sup> ) | MIC (μg/mL) / Inhibition | Reference   |
|----------------------|---------------------------|---------------------------------------|---------------------------------------------|--------------------------|-------------|
| Pure CuO (this work) | Methylene violet (15 ppm) | ~70% in 120 min                       | 0.0055                                      | ~200 μg/mL               | [This work] |

|                                |                                                          |                 |                                      |                                                          |             |
|--------------------------------|----------------------------------------------------------|-----------------|--------------------------------------|----------------------------------------------------------|-------------|
|                                | / <i>Candida albicans</i>                                |                 |                                      |                                                          |             |
| <b>Ni–CuO (this work)</b>      | Methylene violet (15 ppm)<br>/ <i>Candida albicans</i>   | ~82% in 120 min | 0.0098 ( $\approx 2\times$ pure CuO) | ~100 $\mu\text{g/mL}$                                    | [This work] |
| <b>CuO/ZnO (4:6 composite)</b> | Methylene blue (10 ppm)                                  | ~95% in 120 min | 0.0295                               | MIC not reported                                         | [59]        |
| <b>Co–CuO NPs</b>              | Rhodamine B                                              | ~96% in 20 min  | –                                    | MIC not reported                                         | [60]        |
| <b>Zn–CuO NPs</b>              | <i>E. coli</i> , <i>S. aureus</i> , <i>P. aeruginosa</i> | –               | –                                    | Improved inhibition zones vs pure CuO (MIC not reported) | [61]        |