Orbital hybridization induced band offset phenomena in Ni$_x$Cd$_{1-x}$O thin films

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### Table (S1): Calculated and obtained numerical values of different parameters

| Sample name | 2θ Position of (111) peak (degree) | FWHM of (111) peak | 2θ Position of (220) peak (degree) | Effective reduced mass (atomic weight) | Compositional percentage from RBS measurements |
|-------------|-----------------------------------|--------------------|-----------------------------------|----------------------------------------|-----------------------------------------------|
|             |                                   |                    |                                   |                                        | Cd%   | O%   | Ni%   |
| 4Cd         | 33.06                             | 0.42               | 55.42                             | 14.00                                  | 49.8  | 49.2 | 0     |
| 3% Ni       | 33.04                             | 0.60               | 55.43                             | 13.98                                  | 49    | 49   | 1.9   |
| 5% Ni       | 33.10                             | 0.63               | 55.44                             | 13.96                                  | 46.6  | 49.9 | 3.4   |
| 10% Ni      | 33.13                             | 0.88               | 55.51                             | 13.92                                  | 44.3  | 50   | 5.9   |
| 20% Ni      | 33.24                             | 0.87               | 55.66                             | 13.82                                  | 36.5  | 52.9 | 10.6  |
| 40% Ni      | 33.34                             | 1.39               | 56.04                             | 13.60                                  | 24.1  | 51.9 | 24.1  |
| 80% Ni      | n.a.                              | n.a.               | n.a.                              | 13.00                                  | 5.1   | 57.7 | 37.2  |
| 100% Ni     | n.a.                              | n.a.               | n.a.                              | 12.57                                  | 0     | 58.1 | 41.9  |

n.a. = Not Applicable

### Table (S2): Carrier concentration value with increasing Ni doping percentage for Ni<sub>x</sub>Cd<sub>1-x</sub>O thin films

| Sample name | Carrier concentration (/cc) |
|-------------|-----------------------------|
| 4Cd         | -8.400E+19                  |
| 3% Ni       | -6.587E+19                  |
| 5% Ni       | -5.487E+19                  |
| 10% Ni      | -2.196E+19                  |
| 20% Ni      | -1.887E+19                  |
| 40% Ni      | N.A.                        |

Reference: Arkaprava Das *et al.*, Electronic excitation induced anomalous band gap enhancement in Ni<sub>x</sub>Cd<sub>1-x</sub>O thin films; Vacuum 146 (2017) 287-296
Table (S3): Fitting parameters for O 1s, Ni 2p and Cd 3d XPS spectra

| sample                      | Peak position (eV) | area       | fwhm   |
|-----------------------------|-------------------|------------|--------|
| 4Cd (Cd 3d)                 |                   |            |        |
| CdO                         | 403.5             | 58900      | 1.46   |
| CdO₂                        | 404.4             | 22589      | 1.11   |
| 4Cd (O 1s)                  |                   |            |        |
| Cd(OH)₂/CdCO₃               | 530.5             | 10978      | 1.64   |
| CdO                         | 527.9             | 4704       | 0.91   |
| CdO₂                        | 528.8             | 2709       | 1.29   |
| 5% Ni (Cd 3d)               |                   |            |        |
| CdO                         | 403.5             | 58307      | 1.45   |
| CdO₂                        | 404.4             | 22352      | 1.09   |
| 5% Ni (O 1s)                |                   |            |        |
| Cd(OH)₂/CdCO₃               | 530.5             | 10838      | 1.64   |
| CdO                         | 527.9             | 4600       | 0.91   |
| CdO₂                        | 528.8             | 2689       | 1.29   |
| 5% Ni (Ni 2p)               |                   |            |        |
| Ni⁰                         | 851.5             | 197        | 0.8    |
| Ni²⁺                        | 853.6             | 1259       | 3.1    |
| Satellite                   | 859.9             | 1143       | 5.8    |
| Satellite                   | 871.9             | 2198       | 13.9   |
| 10% Ni (Cd 3d)              |                   |            |        |
| CdO                         | 403.4             | 53205      | 1.15   |
| CdO₂                        | 404.3             | 31243      | 1.37   |
| 10% Ni (O 1s)               |                   |            |        |
| Cd(OH)₂/CdCO₃               | 530.6             | 7728       | 1.74   |
| CdO                         | 528.1             | 8263       | 0.93   |
| CdO₂                        | 528.9             | 1982       | 0.94   |
| 10% Ni (Ni 2p)              |                   |            |        |
| Ni⁰                         | 851.6             | 2771       | 1.09   |
| Ni²⁺                        | 853.6             | 5492       | 2.9    |
| Satellite                   | 859.7             | 7844       | 7.3    |
| Satellite                   | 871.1             | 5605       | 6.1    |
| Satellite                   | 878.5             | 3302       | 6.2    |
| 40% Ni (Cd 3d)              |                   |            |        |
| CdO                         | 403.6             | 15848      | 1.24   |
| CdO₂                        | 404.5             | 10064      | 1.23   |
| Compound                  | E (eV) | I (a.u.) | FWHM (eV) |
|---------------------------|--------|----------|-----------|
| Cd(OH)$_2$/CdCO$_3$       | 530.5  | 7646     | 1.86      |
| CdO                       | 528.4  | 4173     | 1.09      |
| CdO$_2$                   | 528.8  | 1958     | 0.84      |
| 40% Ni (Ni 2p)            |        |          |           |
| Ni$^0$                    | 851.8  | 9828     | 0.9       |
| Ni$^{2+}$                 | 852.8  | 19043    | 2.9       |
| Ni$^{3+}$                 | 855.3  | 5381     | 2.4       |
| Satellite                 | 859.4  | 19027    | 6.6       |
| Satellite                 | 872.0  | 19131    | 9         |
| Satellite                 | 879.6  | 4444     | 5         |
| 100% Ni (O 1s)            |        |          |           |
| NiO                       | 529.7  | 12248    | 1.14      |
| Ni(OH)$_2$                | 531.3  | 7300     | 1.92      |
| 100% Ni (Ni 2p)           |        |          |           |
| Ni$^0$                    | 852.5  | 12716    | 0.9       |
| Ni$^{2+}$                 | 854    | 33000    | 2.8       |
| Ni$^{3+}$                 | 856.4  | 13694    | 2.6       |
| Satellite                 | 860.5  | 37560    | 6.8       |
| Satellite                 | 873.3  | 33647    | 9.4       |
| Satellite                 | 880.8  | 8343     | 4.6       |