# Supporting Information

## Identifying Magic-number Structures of Supported Sub-Nano Ni Cluster and the Influence of Hydrogen Coverage: A Density Functional Theory Based Particle Swarm Optimization Investigation

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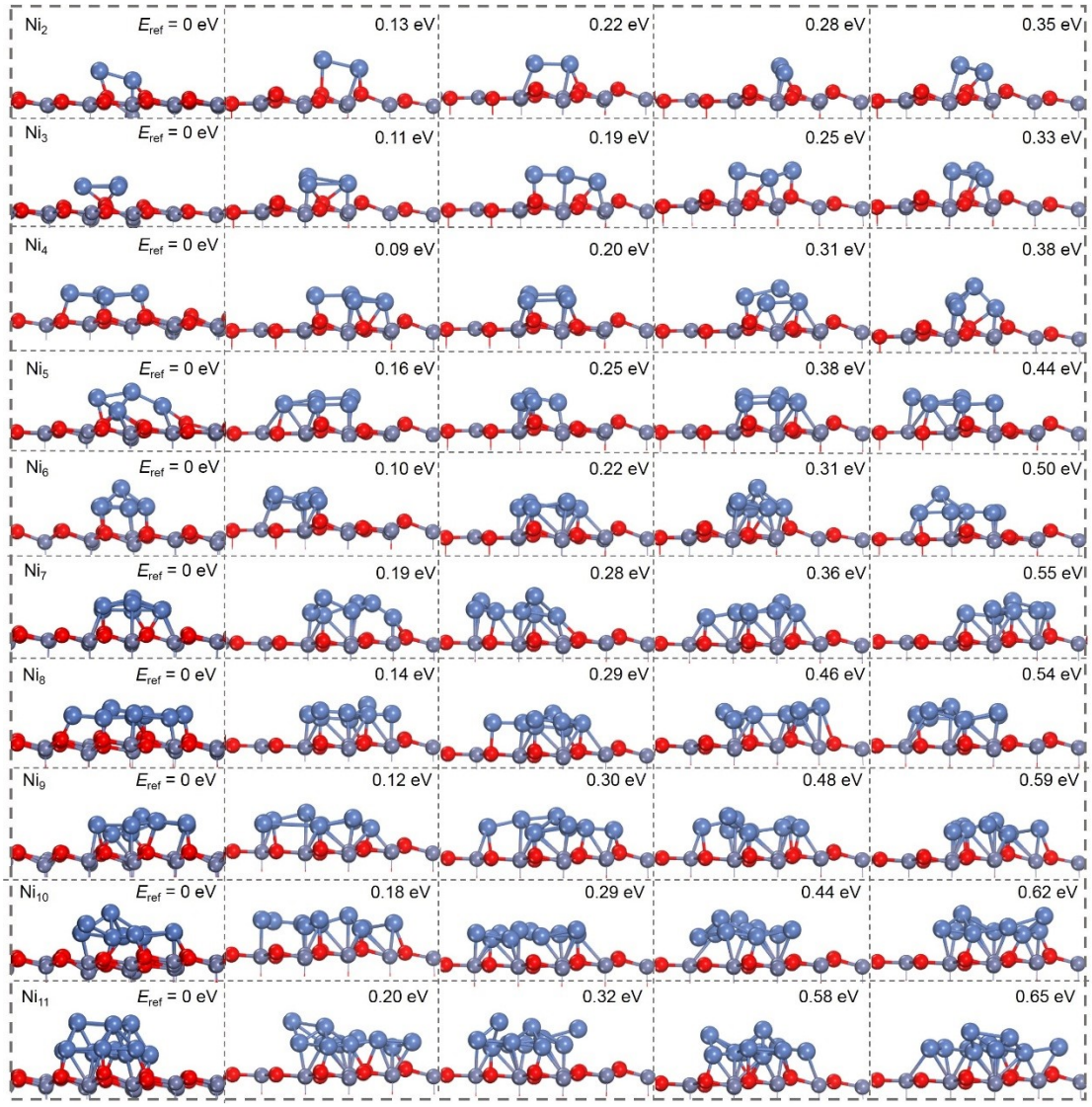


**Figure S1**. Five lowest-energy structures of the $Ni_n$ (n = 2–11) cluster on ZnO($000\bar{1}$). The most stable ones are chosen to represent the global minimum geometries for each cluster, and the corresponding total energies are taken as the energy reference ($E_{ref}$, eV).

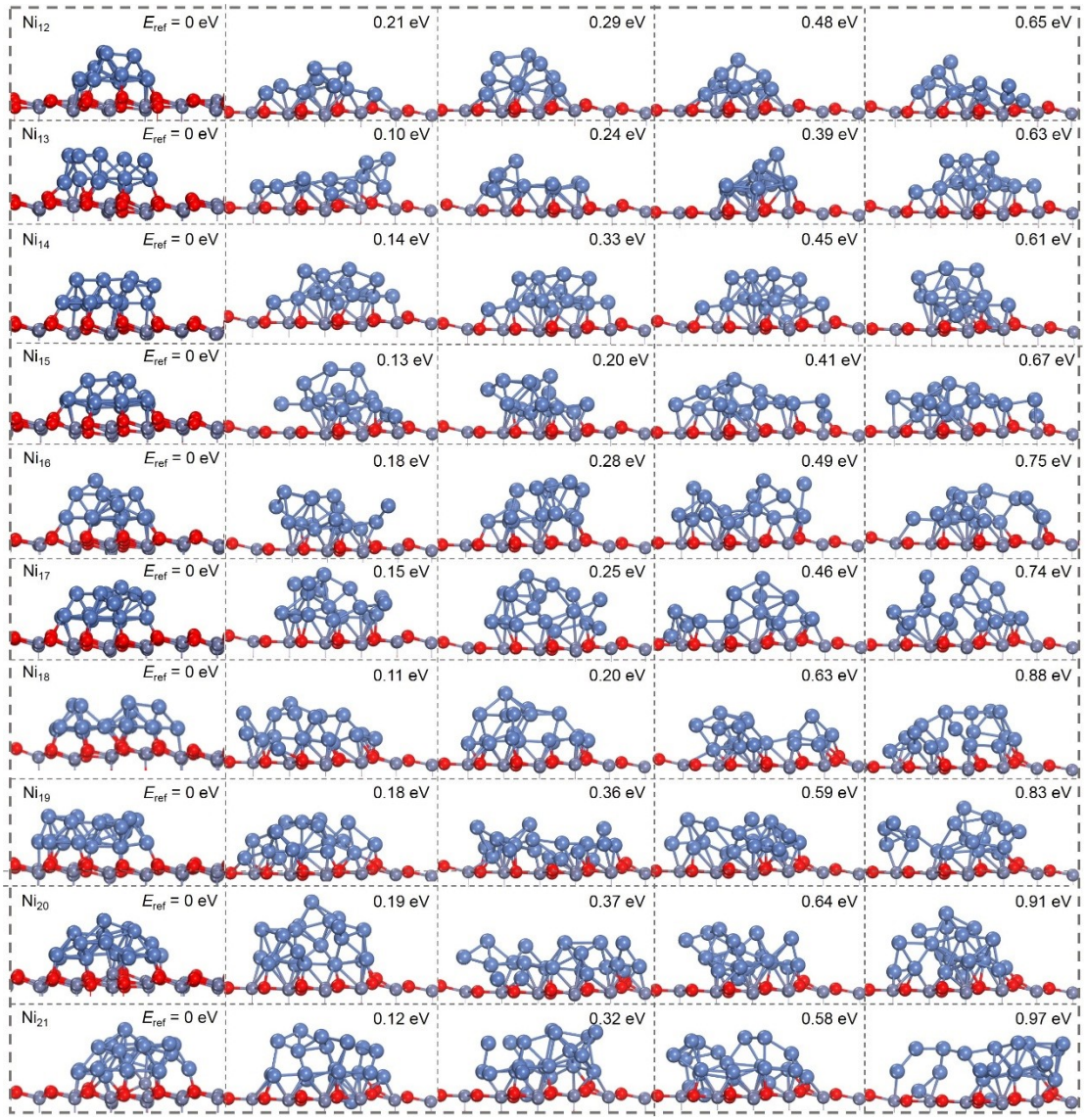


**Figure S2**. Five lowest-energy structures of the $Ni_n$ (n = 12–21) cluster on ZnO($000\bar{1}$). The most stable ones are chosen to represent the global minimum geometries for each cluster, and the corresponding total energies are taken as the energy reference ($E_{ref}$, eV).

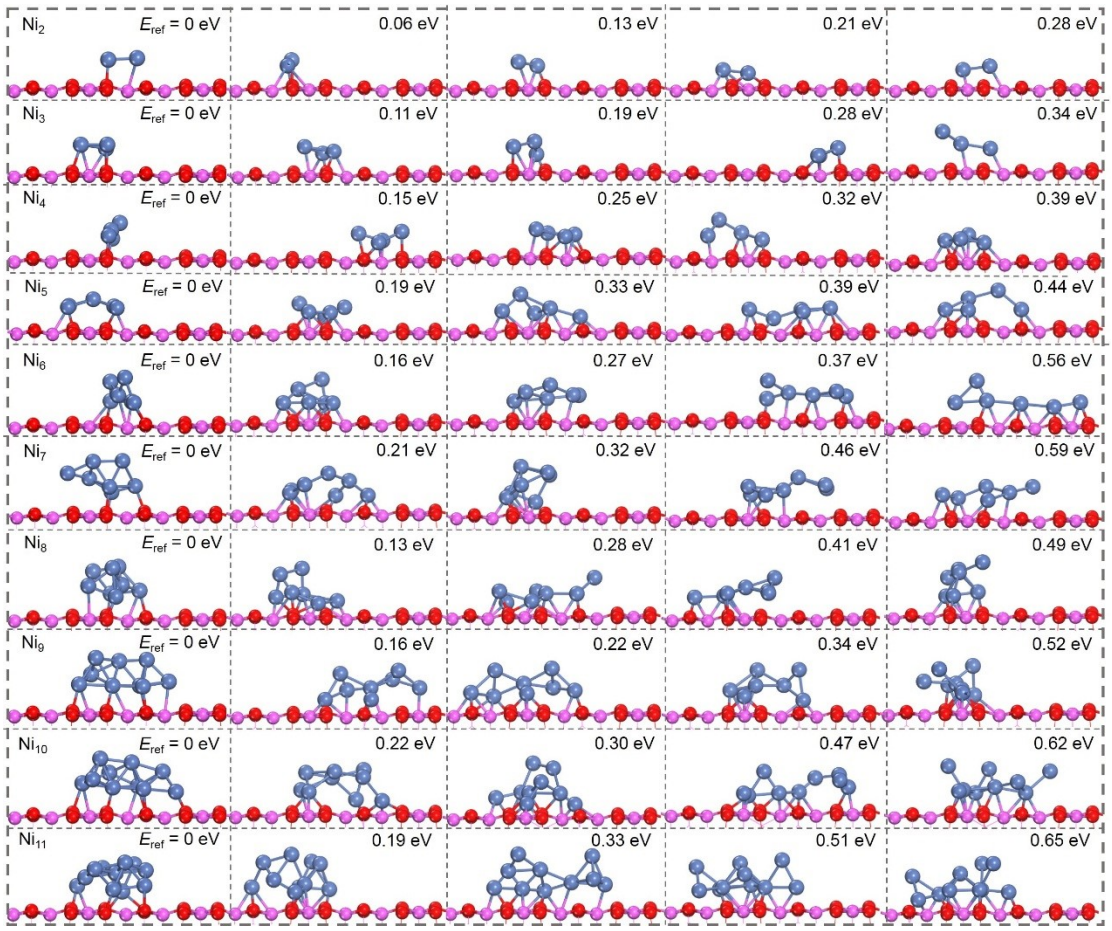


**Figure S3**. Five lowest-energy structures of the $Ni_n$ (n = 2–11) cluster on γ-$Al_2O_3$(100). The most stable ones are chosen to represent the global minimum geometries for each cluster, and the corresponding total energies are taken as the energy reference ($E_{ref}$, eV).

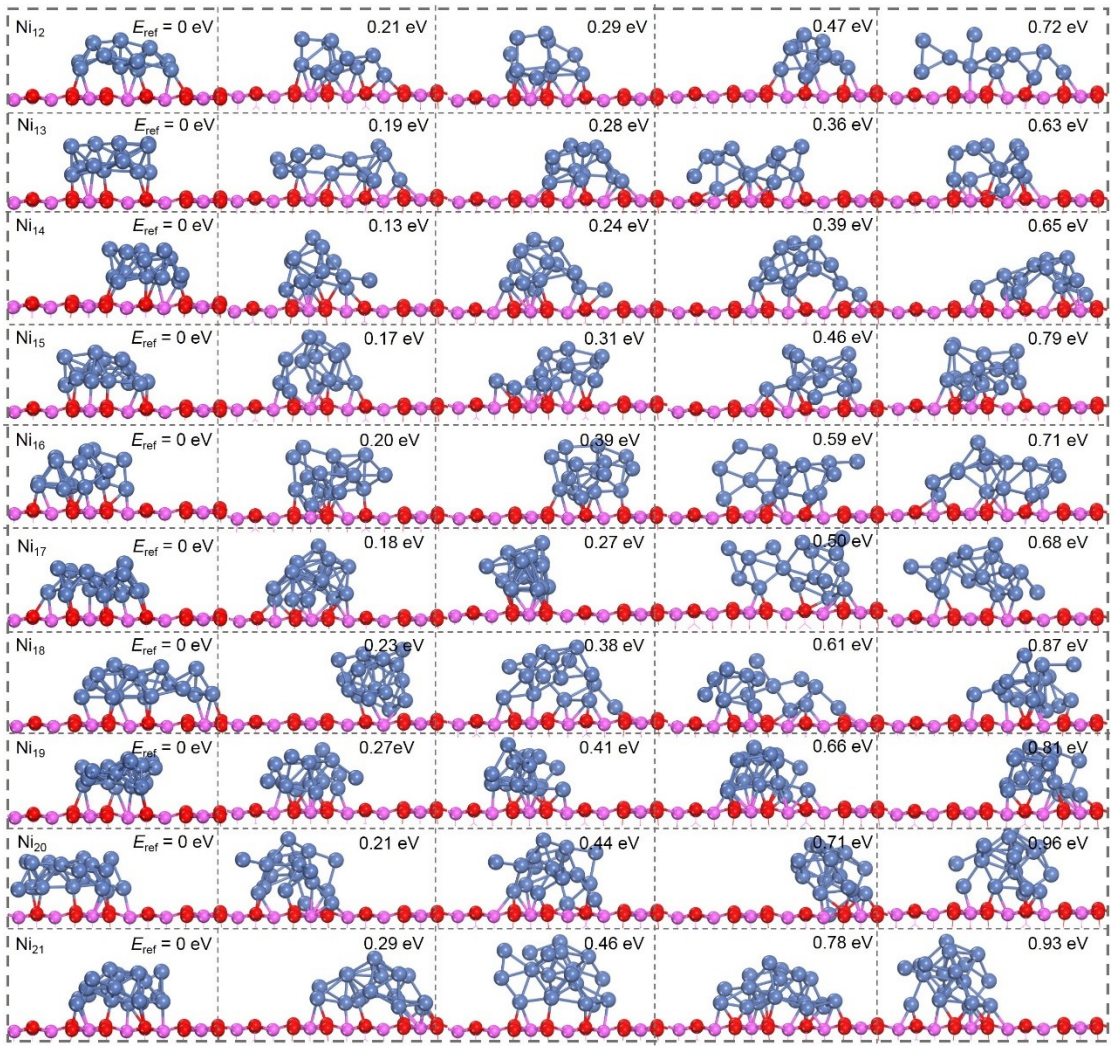


**Figure S4**. Five lowest-energy structures of the $Ni_n$ (n = 12–21) cluster on γ-$Al_2O_3$(100). The most stable ones are chosen to represent the global minimum geometries for each cluster, and the corresponding total energies are taken as the energy reference ($E_{ref}$, eV).

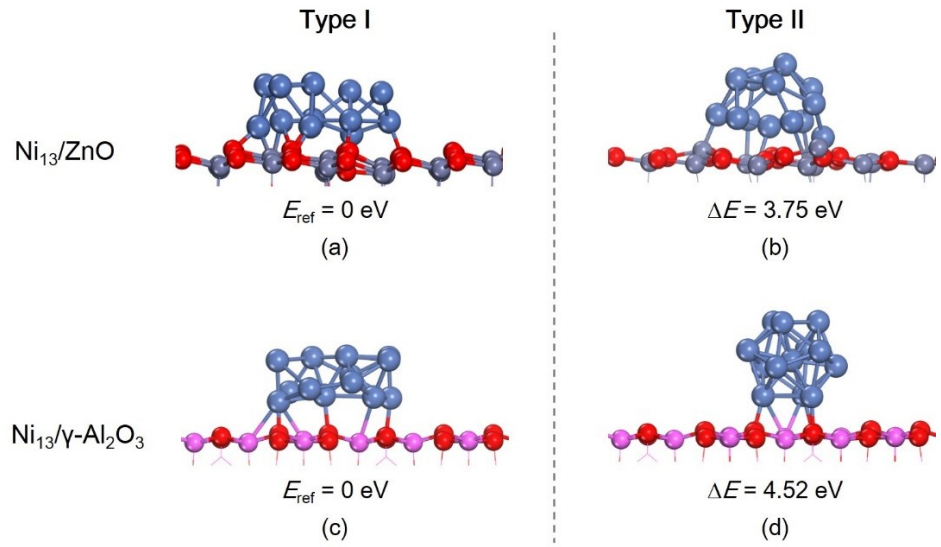


**Figure S5**. Two types of $Ni_{13}$/ZnO and $Ni_{13}$/γ-$Al_2O_3$ models. Type I: $Ni_{13}$/ZnO (a) and $Ni_{13}$/γ-$Al_2O_3$ (c) models are searched and optimized by the DFT based PSO methods. Type II: $Ni_{13}$/ZnO (b) and $Ni_{13}$/γ-$Al_2O_3$ (d) models are constructed by direct deposition of the most stable gas-phase magic $Ni_{13}$ cluster on ZnO($000\bar{1}$) and γ-$Al_2O_3$(100), respectively. The total energies of Type I models are taken as the energy reference ($E_{ref}$, eV).

**Table S1. Average uncoordinated bonds (AUB) of gas-phase Ni clusters.**

| | AUB | | AUB |
|---|---|---|---|
| $Ni_2$ | 11.00 | $Ni_{12}$ | 6.00 |
| $Ni_3$ | 10.00 | $Ni_{13}$ | 5.64 |
| $Ni_4$ | 9.00 | $Ni_{14}$ | 5.60 |
| $Ni_5$ | 8.00 | $Ni_{15}$ | 5.57 |
| $Ni_6$ | 8.00 | $Ni_{16}$ | 5.56 |
| $Ni_7$ | 7.50 | $Ni_{17}$ | 5.56 |
| $Ni_8$ | 7.42 | $Ni_{18}$ | 5.50 |
| $Ni_9$ | 6.89 | $Ni_{19}$ | 5.36 |
| $Ni_{10}$ | 6.7 | $Ni_{20}$ | 5.04 |
| $Ni_{11}$ | 6.36 | $Ni_{21}$ | 5.00 |

**Table S2. Comparison between the D3 corrected and uncorrected energies (eV) for the $Ni_{11}H_x$ (x = 2, 4, 6, 8, 10, 12) clusters on ZnO and γ-$Al_2O_3$ surfaces.**

| | ZnO | | $Al_2O_3$ | |
|---|---|---|---|---|
| | uncorrected | corrected | uncorrected | corrected |
| $Ni_{11}H_2$ | –477.48 | –480.23 | –881.12 | –885.11 |
| $Ni_{11}H_4$ | –481.55 | –484.36 | –887.96 | –891.94 |
| $Ni_{11}H_6$ | –490.84 | –493.67 | –896.45 | –900.52 |
| $Ni_{11}H_8$ | –499.87 | –502.79 | –902.48 | –906.61 |
| $Ni_{11}H_{10}$ | –508.11 | –511.12 | –909.53 | –913.75 |
| $Ni_{11}H_{12}$ | –516.63 | –519.71 | –916.74 | –920.91 |