Supplementary Information

# NiO nanoparticle surface energy studies by the first principles calculation

*Junxiang Xiang[1,3], Bin Xiang[1,3*], Xudong Cui[1,2,*]*

1. Photonic Technology Research and Development Center, Quanzhou Normal University, No 398, Donghai Main Street, Quanzhou, Fujian 362000, China
2. Sichuan New Materials Research Center, Institute of Chemical Materials, CAEP, Chengdu, Sichuan, 610200 China
3. Department of Materials Science & Engineering, CAS key Lab of Materials for Energy Conversion, Synergetic Innovation Center of Quantum Information & Quantum Physics, University of Science and Technology of China, Hefei, Anhui, 230026, China

*E-mail: xudcui@caep.cn; binxiang@ustc.edu.cn

Table S1.

Lattice constant, bulk modulus, band gap, magnetic moment, and surface energy of NiO from different GGA methods and experimental results. GGA is the GGA-PBE method, and SGGA is spin-polarized GGA-PBE method, and GGA+U is spin-polarized GGA-PBE method with Hubbard U correction for 3d electrons.

| | GGA | SGGA | GGA+U | Experiment |
|---|---|---|---|---|
| Lattice Constant (Å) | 4.18886 | 4.18898 | 4.29895 | 4.17 |
| Bulk Modulus (GPa) | 205.63 | 205.11 | 122.76 | 205 |
| Band Gap (eV) | 0 | 0 | 0 | 4.3 |
| Magnetic Moment (μB) | - | 0 | 1.76 | 1.90 |
| (001) Surface Energy ($J/m^2$) | 0.60 | 0.98 | 0.10 | - |
| (110) Surface Energy ($J/m^2$) | 1.15 | 2.35 | 1.43 | - |
| (111) Surface Energy ($J/m^2$) | 2.03 | 4.40 | 5.29 | - |

The calculations using GGA or SGGA methods give out similar results of lattice constant and bulk modulus well consistent with experimental results. GGA-Spin+U method gives out a larger lattice constant than experimental result by about 3% and a much smaller bulk modulus than experimental result by about 40%. Thus, GGA method without considering spin effect can appropriately predict stable bulk NiO.

The surface energy of NiO (100), (110), (111) calculated through the three method has the same trend. The consistency make it reasonable to discard the spin polarization and Hubbard correction in the surface energy calculations in our work.

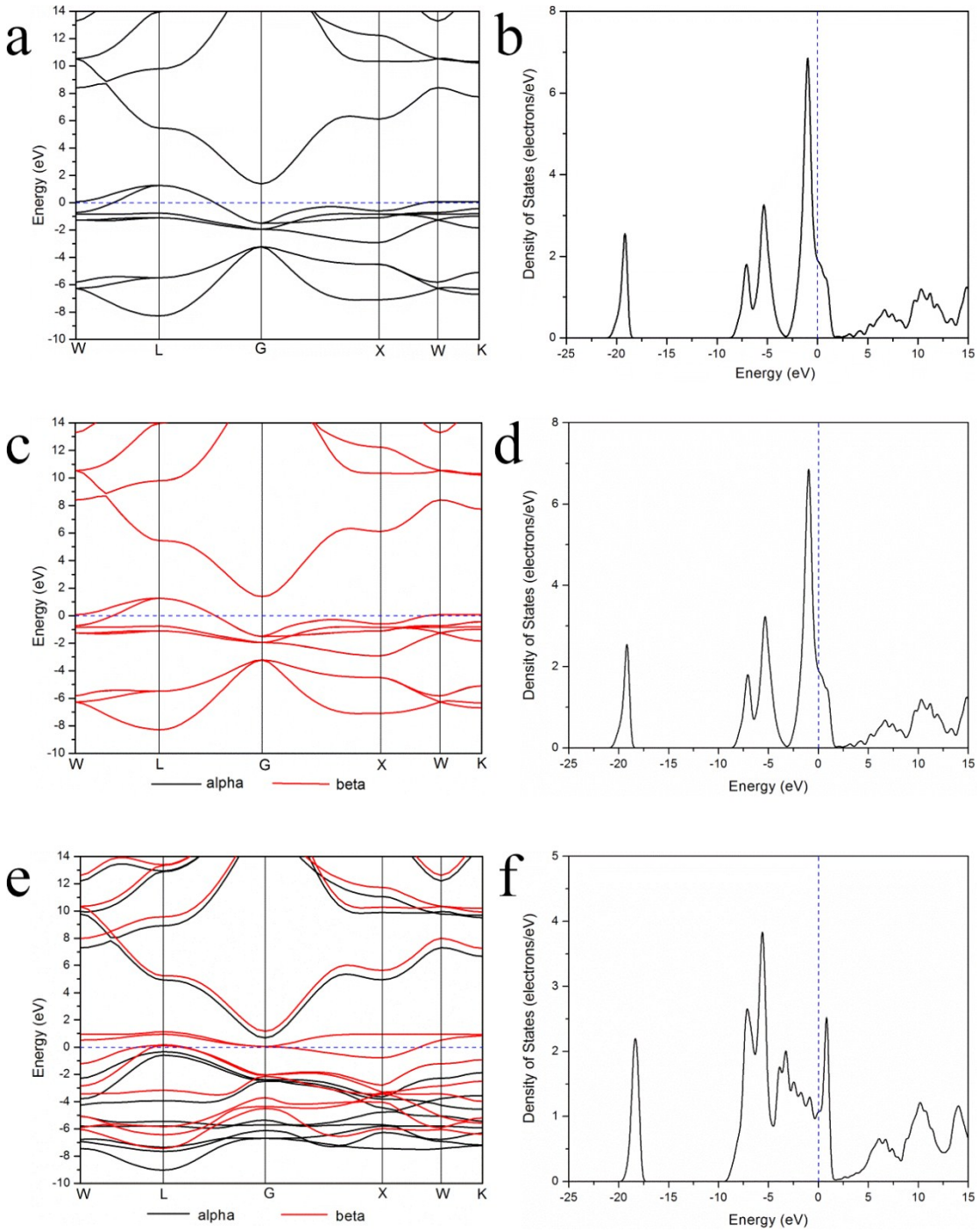


**Figure S1.** Band structure (a) and total density of states (b) of GGA-PBE calculated bulk NiO. Band structure (c) and total density of states (d) of SGGA calculated bulk NiO. Band structure (e) and total density of states (f) of thorough GGA+U calculated bulk NiO.

GGA, SGGA, and GGA+U calculations give out the band structure and total denstity of states of this calculation are showed in **Figure S1.** The Fermi levels of the three calculations all get into the valence band, indicating all three methods predicted a metallic property for bulk

NiO. Meanwhile, SGGA method predicted bulk NiO having 0 $\mu_B$ magnetic moment, while GGA+U predicted it having 1.76 $\mu_B$ magnetic moment close to 1.90 $\mu_B$ of the experimental result.

In conclusion, GGA, SGGA, and GGA+U methods failed to evaluate the correct band gap of bulk NiO represented by rock salt crystal structure. GGA and SGGA methods gave experimental-consistent results of lattice parameters and bulk modulus. GGA+U method is superior in magnetic calculation of NiO. All three methods predicted the same tendency of surface energy of NiO (100), (110), and (111).