Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Structural and Electronic Changes in the $Ni_{13}@Ag_{42}$ Nanoparticle Under Surface Oxidation. The Role of the Silver Coating.

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I. ELECTRONIC PROPERTIES

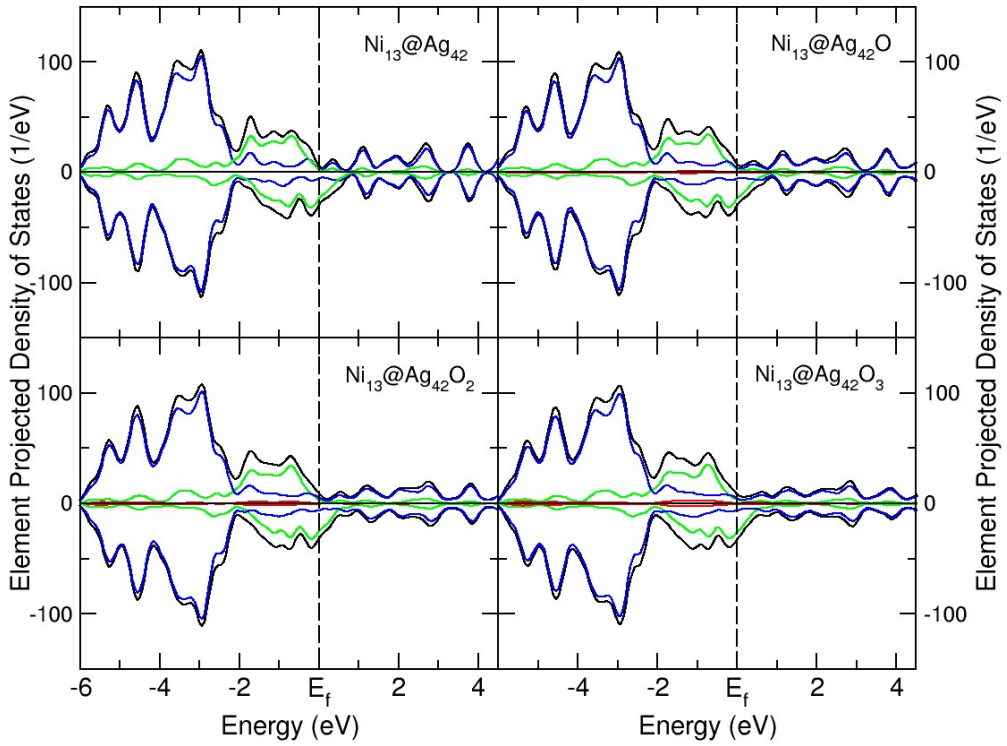

FIG. 1. (Color online) The density of states (DOS) and partial density of states (PDOS) are shown for the putative ground state atomic configurations of Ni13Ag42O$_m$ with $m = 0$ to 3. The DOS is represented in black, while the PDOS of silver, nickel, and oxygen atoms are depicted in blue, green, and red, respectively.

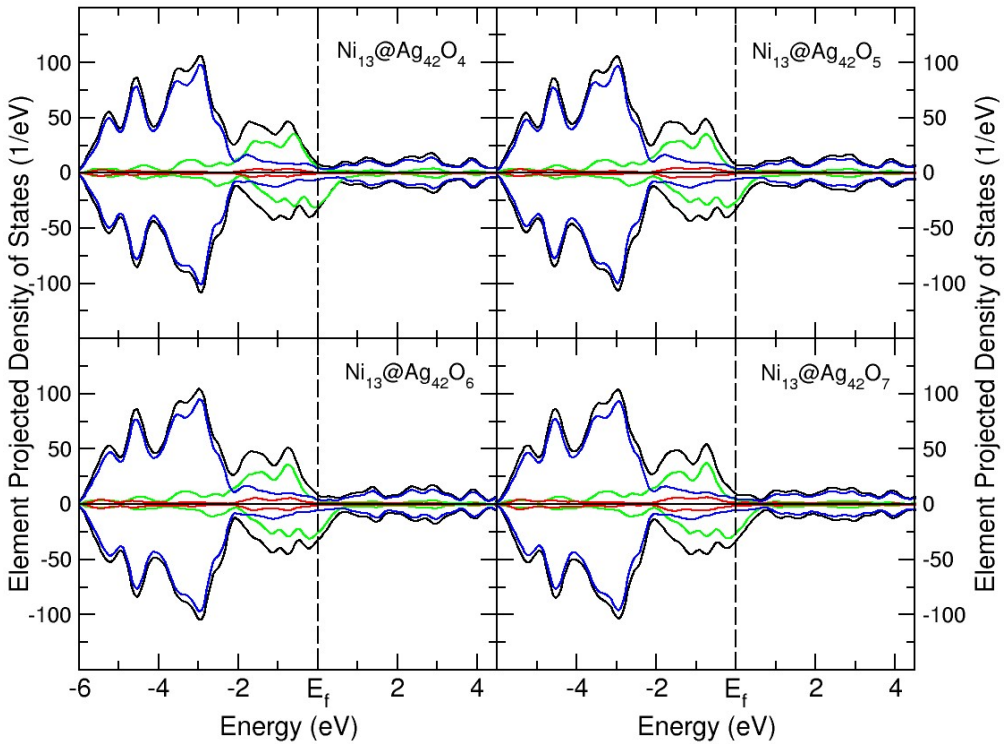

FIG. 2. (Color online) The density of states (DOS) and partial density of states (PDOS) are shown for the putative ground state atomic configurations of Ni13Ag42O$_m$ with $m = 4$ to 7. The DOS is represented in black, while the PDOS of silver, nickel, and oxygen atoms are depicted in blue, green, and red, respectively.

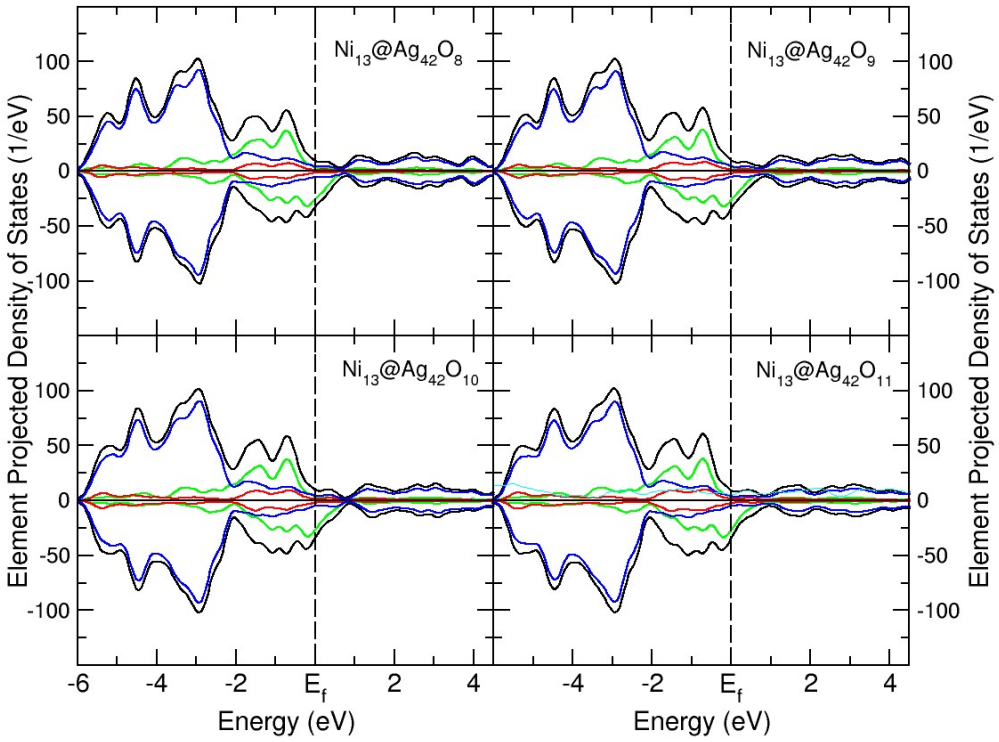

FIG. 3. (Color online) The density of states (DOS) and partial density of states (PDOS) are shown for the putative ground state atomic configurations of Ni13Ag42O$_m$ with $m = 8$ to 11. The DOS is represented in black, while the PDOS of silver, nickel, and oxygen atoms are depicted in blue, green, and red, respectively.

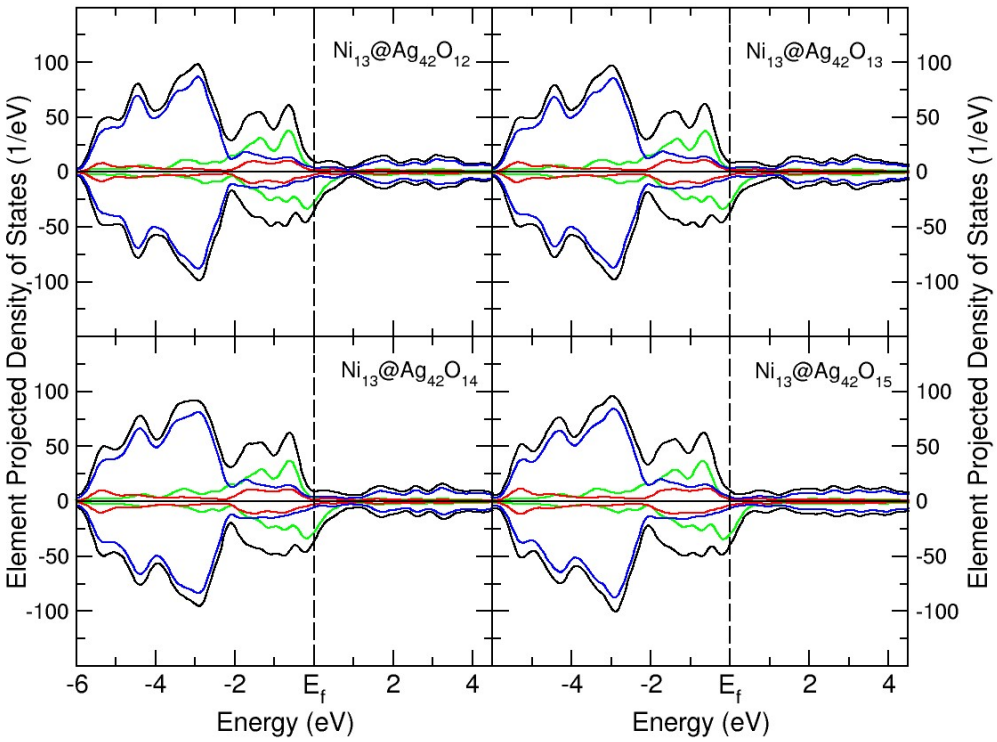

FIG. 4. (Color online) The density of states (DOS) and partial density of states (PDOS) are shown for the putative ground state atomic configurations of Ni13Ag42O$_m$ with m = 12 to 15. The DOS is represented in black, while the PDOS of silver, nickel, and oxygen atoms are depicted in blue, green, and red, respectively.

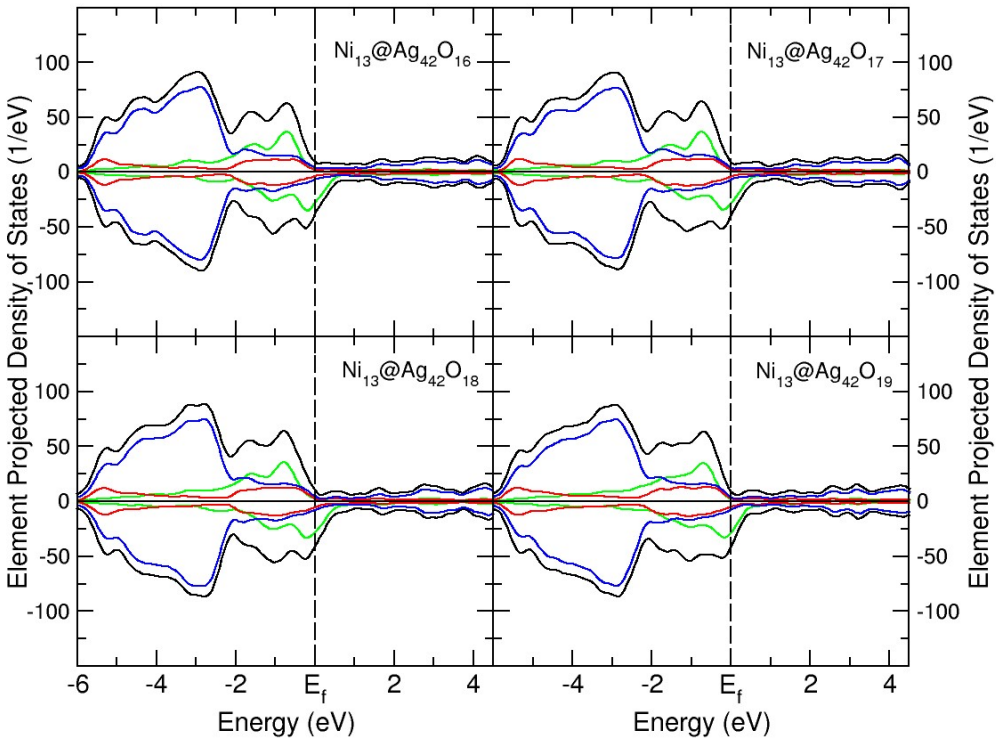

FIG. 5. (Color online) The density of states (DOS) and partial density of states (PDOS) are shown for the putative ground state atomic configurations of Ni13Ag42O$_m$ with $m = 16$ to 19. The DOS is represented in black, while the PDOS of silver, nickel, and oxygen atoms are depicted in blue, green, and red, respectively.

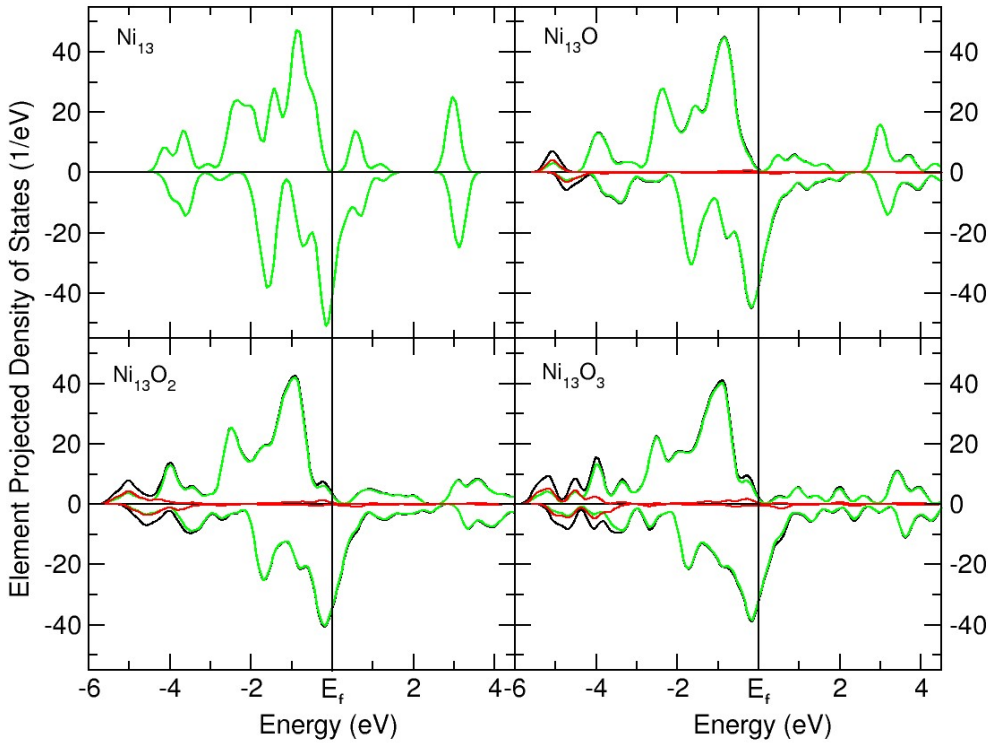

FIG. 6. (Color online) The density of states (DOS) and partial density of states (PDOS) are shown for the putative ground state atomic configurations of Ni13O$_m$ with $m = 0$ to 3. The DOS is represented in black, while the PDOS of nickel, and oxygen atoms are depicted in green, and red, respectively.

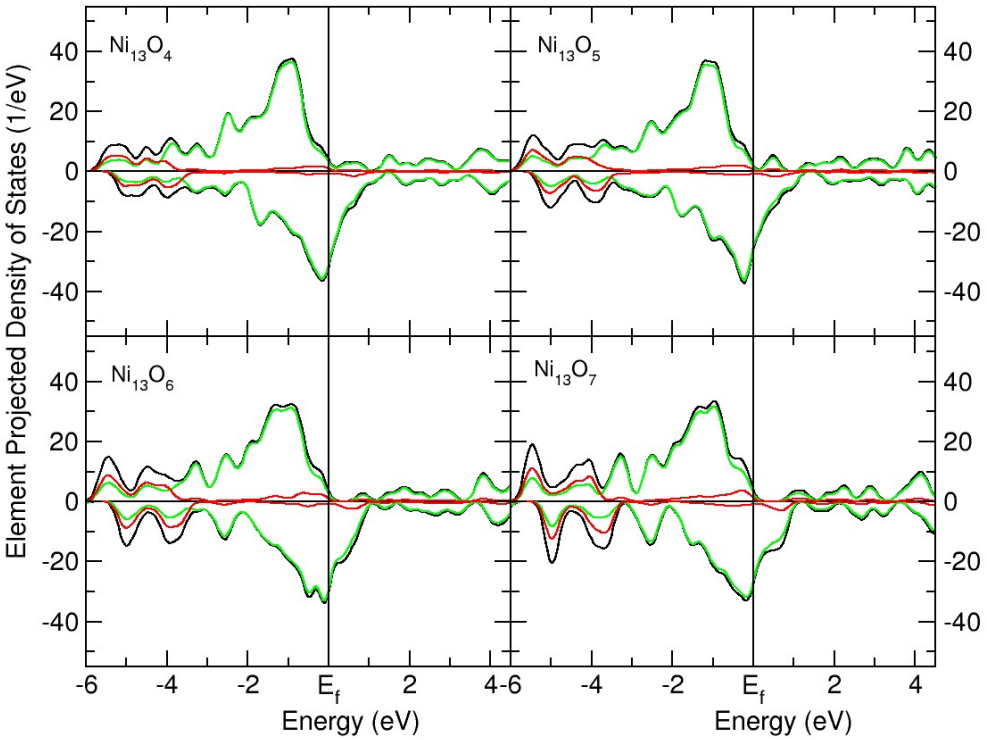

FIG. 7. (Color online) The density of states (DOS) and partial density of states (PDOS) are shown for the putative ground state atomic configurations of Ni13O$_m$ with $m = 4$ to 7. The DOS is represented in black, while the PDOS of nickel, and oxygen atoms are depicted in green, and red, respectively.

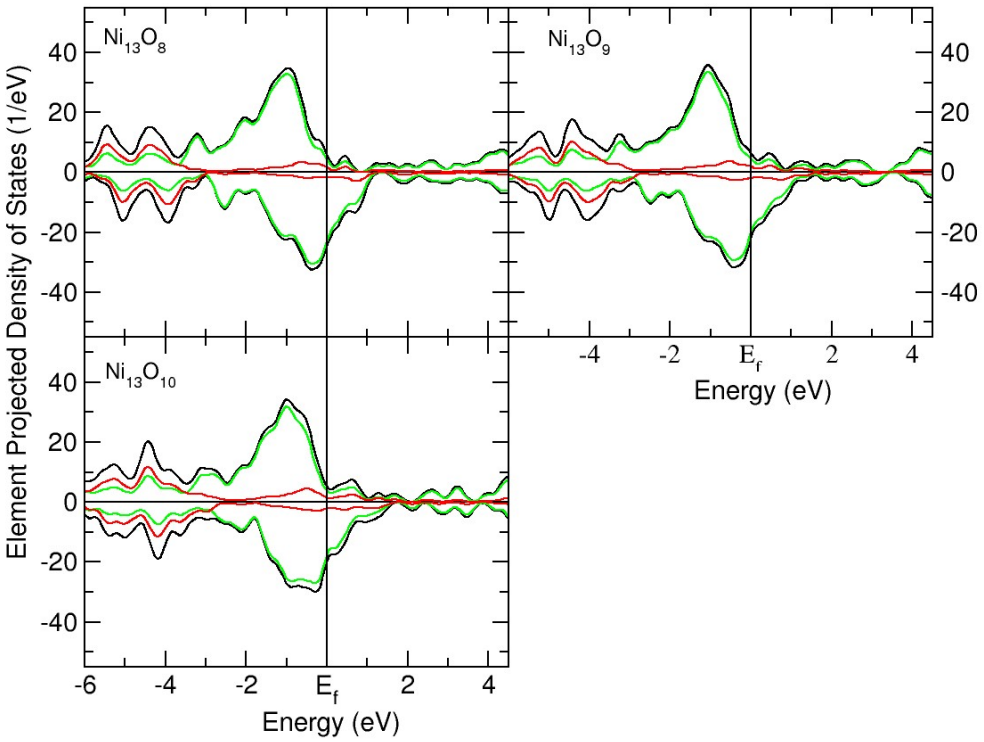

FIG. 8. (Color online) The density of states (DOS) and partial density of states (PDOS) are shown for the putative ground state atomic configurations of Ni13O$_m$ with m = 8 to 10. The DOS is represented in black, while the PDOS of nickel, and oxygen atoms are depicted in green, and red, respectively.

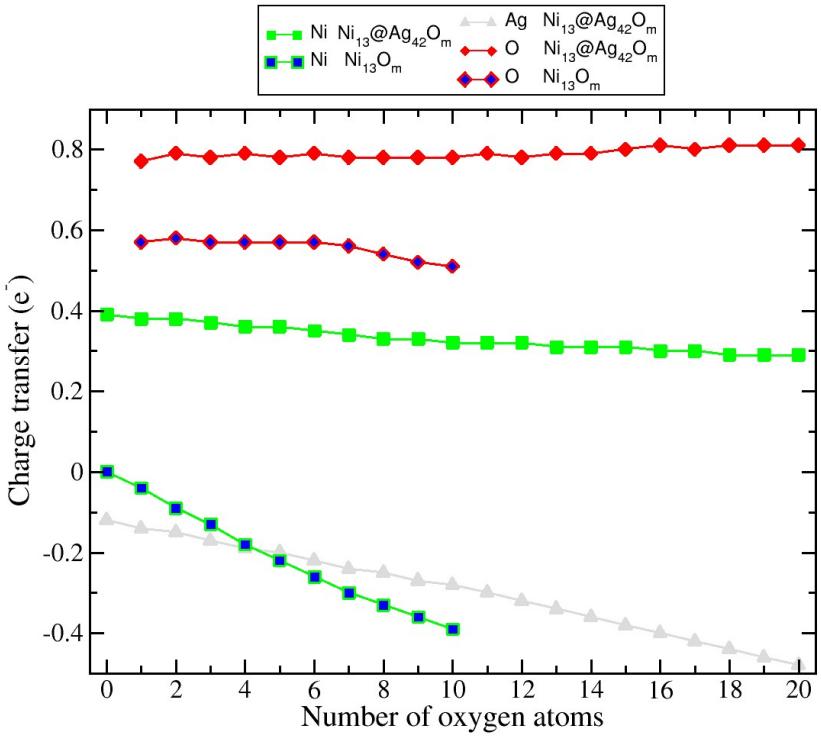

FIG. 9. (Color online) Putative ground state atomic configurations of $Ni_{13}O_m$ with m= 1 to 10.