SUPPORTING INFORMATION

CO adsorption, oxidation and carbonate formation mechanisms on Fe3O4 surfaces

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Figure S1. Configurations of least stable CO adsorption and oxidation on Fe$_{tet1}$ termination

(a) -0.41  (b) 1.11  (c) 0.40  (d) -0.19
(e) 0.01

Figure S2. Configurations of least stable CO adsorption and oxidation on Fe$_{oct2}$ termination

(a) -1.54  (b) -0.57  (c) -0.56  (d) -0.38
(h) -1.94  (i) -1.26  (k) -0.98  (n) -2.04
(o) -1.83
Figure S3. Configurations of least stable CO adsorption, oxidation and carbonate on Fe$_3$O$_4$(110) A layer.

Figure S4. Configurations of least stable CO adsorption and oxidation on Fe$_3$O$_4$(110) B layer.
Figure S5. Configurations of least stable CO adsorption, oxidation and carbonate on on Fe₃O₄(001) B termination.