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Addition/Correction

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Correction to "Surface Structure and Environment-Dependent Hydroxylation of the Nonpolar Hematite (100) from Density Functional Theory Modeling"

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Due to mistakes in calculating the temperature-dependent chemical potential of water vapor, the phase boundaries in the phase-diagrams shown in Figures 5, 6, and 8 were incorrect. The correct figures are as follows. The conclusions remain unchanged with the corrections.

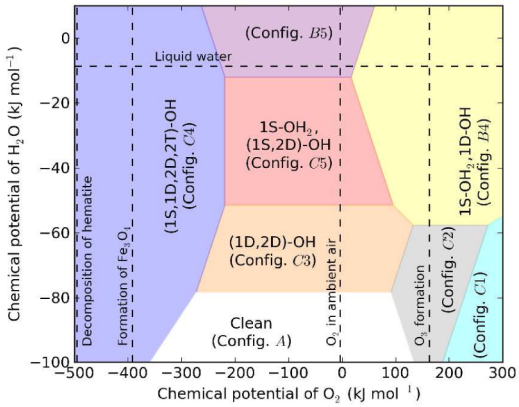

Figure 5. Relative stability of the surface configurations of hematite (100) at 298.15 K. The vertial dashed lines, from left to right, correspond to the chemical potential of hematite reduction to form bulk Fe, hematite reduction to form magnetite, O_2 in atmospheric air, and the formation of ozone (O_3) at thermodynamic standard state. The chemical potential of liquid water is marked with a horizontal line. Refer to the texts and Supporting Information for the notations about the surface terminations.

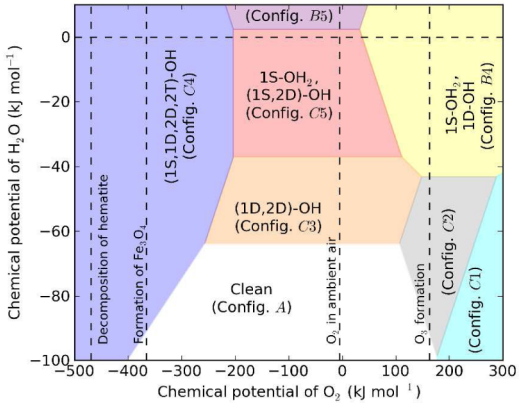

Figure 6. Relative stability of the surface configurations of hematite (100) at 373.15 K. Refer to the caption of Figure 5 for the notations and marks.

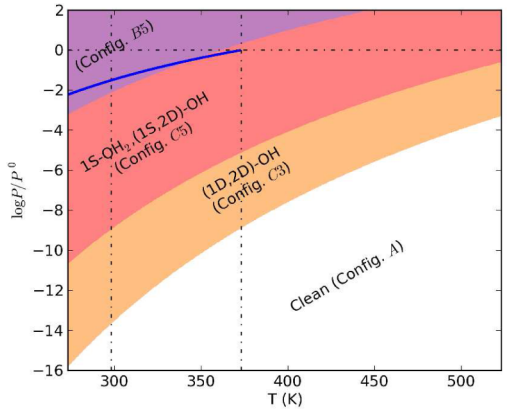

Figure 8. Temperature-dependent phase diagram of the (100) surface. The bold blue line represents the saturated vapor pressure of water in the temperature range from 273.15 to 373.15 K. The vertical dash-dotted lines mark 298.15 K (the standard temperature) and 373.15 K (the boiling temperature of water under 1 atm). The horizontal dashdotted line marks the standard pressure (1 atm).

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