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Addition/Correction

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Correction to "Molecular-Level Details about Liquid H_2O Interactions with CO and Sugar Alcohol Adsorbates on Pt(111) Calculated Using Density Functional Theory and Molecular Dynamics"

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We have become aware of errors in the reported numbers of water molecules hydrogen-bonded to the adsorbates tested, and we report corrected numbers here. The corrected values for CO are 1.3 ± 0.5 hydrogen-bonded water molecules; i.e., 13 total hydrogen bonds were found in the 10 configurations considered, with an average $O_{H_2O}-O_{CO}$ distance of 2.93 ± 0.09 Å and an average O−O−H angle of 17.4 ± 4.5°. The corrected values for CH_2OH are 1.8 ± 0.3 hydrogen-bonded water molecules, with an average $O_{H_2O}-O_{CH_2OH}$ distance of 2.80 ± 0.08 Å and an average O−O−H angle of 13.5 ± 2.8°. The corrected values for $C_3H_7O_3$ are 4.0 ± 0.7 hydrogen-bonded water molecules, with an average $O_{C_3H_7O_3}-O_{H_2O}$ distance of 2.86 ± 0.08 Å and an average O−O−H angle of 14.1 ± 2.7°. Figure 2 has been updated to include these values, as shown below. Additionally, any conclusions made regarding the insufficiency of our model for $C_3H_7O_3$ are no longer valid, as our corrected values show that this method is sufficient for all three adsorbates tested.

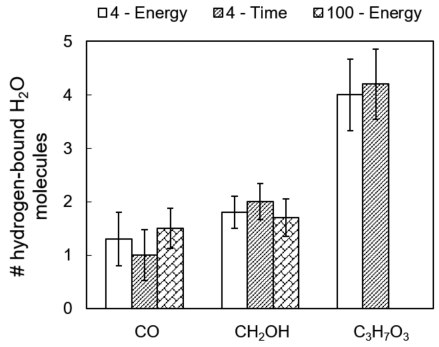

Figure 2. Number of H_2O molecules that hydrogen-bond to CO, CH_2OH, and $C_3H_7O_3$ adsorbates using the "energy" and "time" sampling methods. The numbers "4" and "100" indicate the number of "layers" of ice in the starting configurations. Error bars are 95% confidence intervals.

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