Supporting Information for:

What can Raman spectroscopy really say about the adsorbed CO on roughened Cu electrodes in CO_2 electroreduction conditions?

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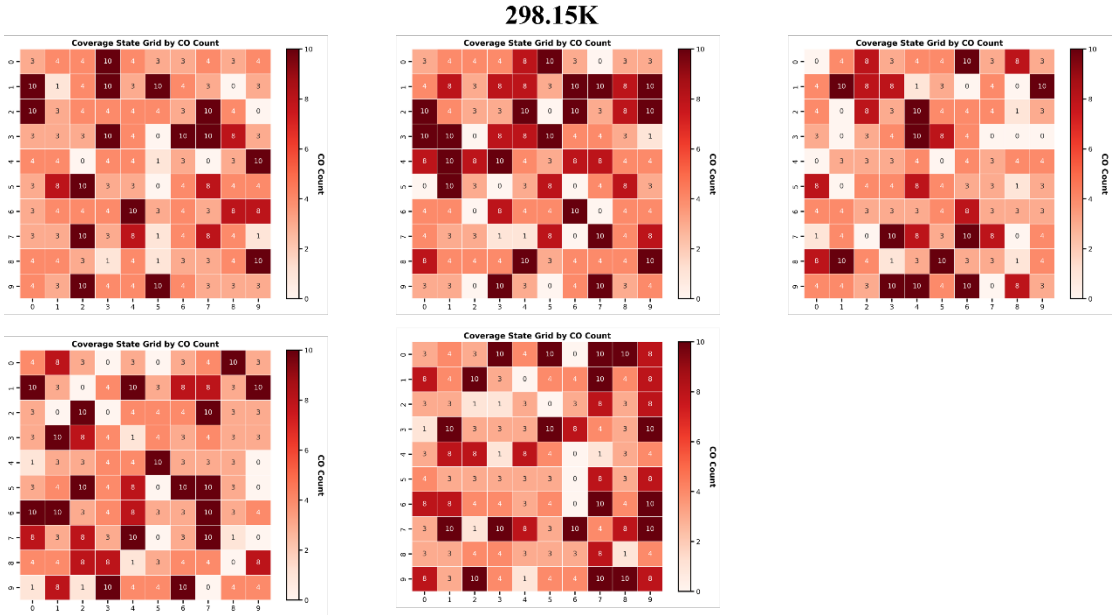

Figure 1S. Final configuration distributions obtained from KMC simulations at 298.15 K under an applied potential of –1.1 V_{RHE}. Five independent simulations were performed, they show the final states from each run. Each grid cell represents a distinct surface structure, with the number inside indicating the count of adsorbed *CO molecules. Darker colors correspond to higher *CO coverages.

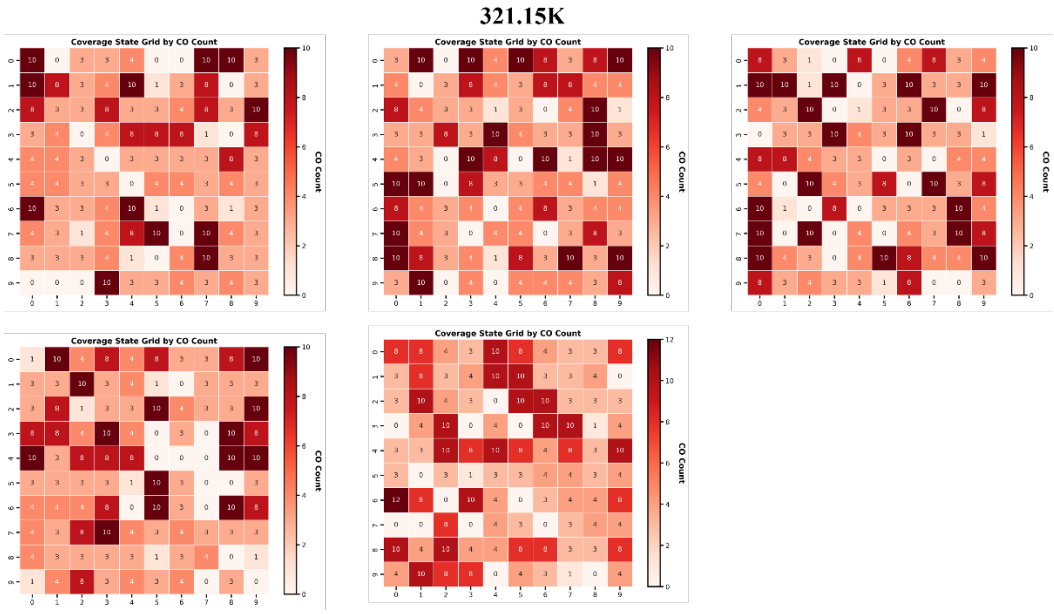

Figure 2S. Final configuration distributions obtained from KMC simulations at 321.15 K under an applied potential of –1.1 V_{RHE}. Five independent simulations were performed, they show the final states from each run. Each grid cell represents a distinct surface structure, with the number inside indicating the count of adsorbed *CO molecules. Darker colors correspond to higher *CO coverages.

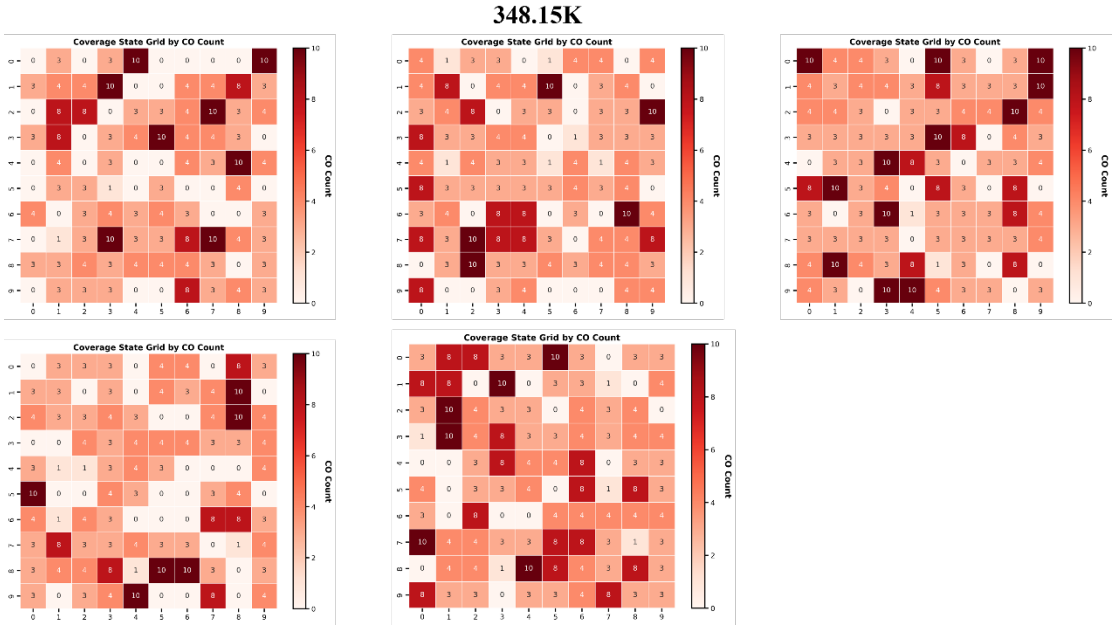

Figure 3S. Final configuration distributions obtained from KMC simulations at 348.15 K under an applied potential of –1.1 V_{RHE}. Five independent simulations were performed, they show the final states from each run. Each grid cell represents a distinct surface structure, with the number inside indicating the count of adsorbed *CO molecules. Darker colors correspond to higher *CO coverages.

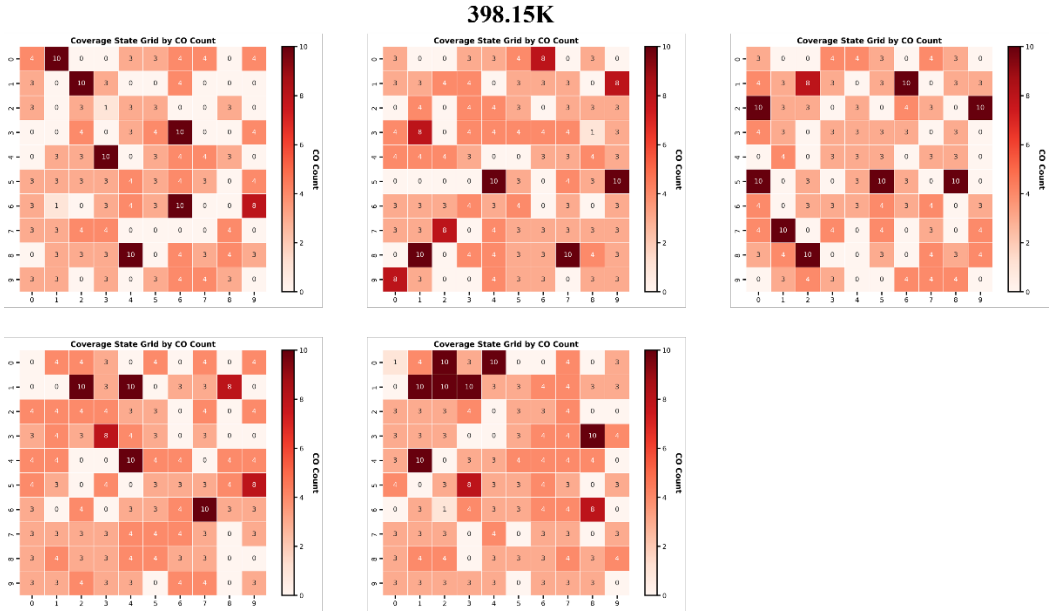

Figure 4S. Final configuration distributions obtained from KMC simulations at 398.15 K under an applied potential of –1.1 V_{RHE}. Five independent simulations were performed, they show the final states from each run. Each grid cell represents a distinct surface structure, with the number inside indicating the count of adsorbed *CO molecules. Darker colors correspond to higher *CO coverages.

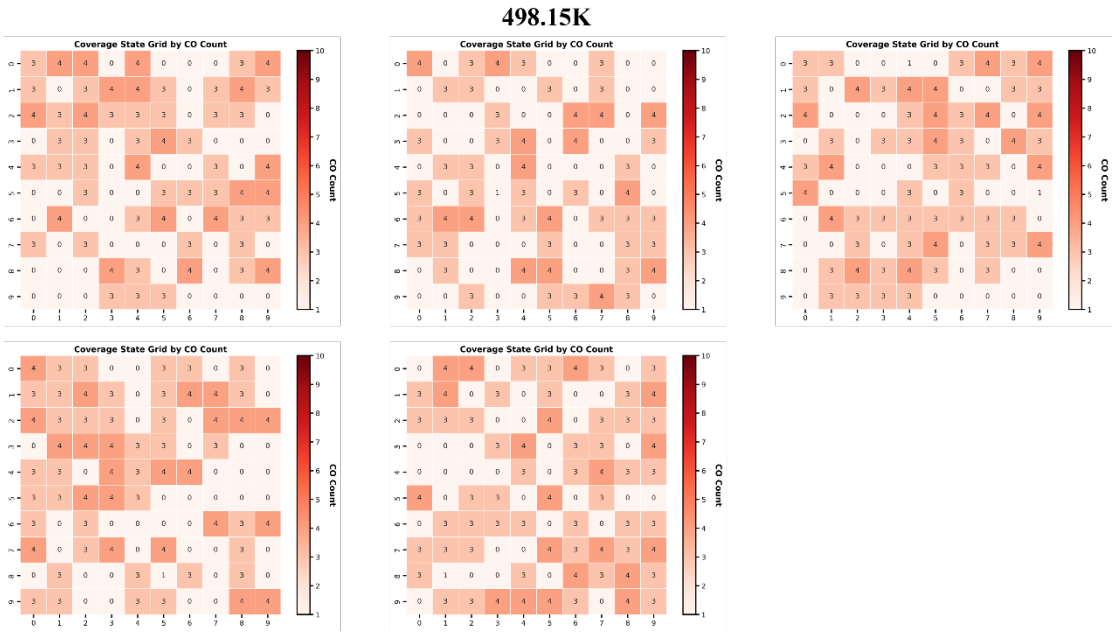

Figure 5S. Final configuration distributions obtained from KMC simulations at 498.15 K under an applied potential of –1.1 V_{RHE}. Five independent simulations were performed, they show the final states from each run. Each grid cell represents a distinct surface structure, with the number inside indicating the count of adsorbed *CO molecules. Darker colors correspond to higher *CO coverages.

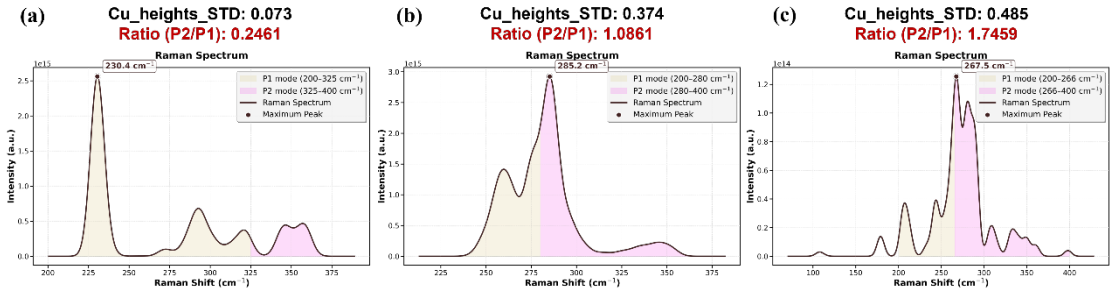

Figure 6S. Raman spectra for the three structures shown in Figure 2, each exhibiting different standard deviations of top-layer Cu atom heights at a fixed CO coverage of 0.33 ML. The corresponding Raman intensity ratios (P_2/P_1) are indicated for each structure.

All structures used in this study are available online at https://github.com/alexandrova-lab-ucla/Article-Data