Correction: Surface heterogeneity and inhomogeneous broadening of vibrational line profiles

Skandar Taj, Diane Baird, Alexander Rosu-Finsen and Martin R. S. McCoustra*


Ref. 1 considered the profile of the C=O stretching vibration for carbon monoxide (CO) adsorbed in sub-monolayer quantities on amorphous silica (aSiO$_2$) and on porous amorphous solid water (p-ASW). The paper presented the hypothesis that the C=O stretching frequency is sensitive to the interaction experienced by the CO on the surface and that this heterogeneity can be recovered from temperature programmed desorption (TPD) analysis. In the paper, we reported TPD inversion for CO on aSiO$_2$ from which we derived the relevant probability distribution $P(E_{\text{des}})$ reflecting the interaction of CO with the aSiO$_2$. The data for p-ASW were taken from work by Kay and colleagues as cited in the paper. Simulations of the heterogeneously broadened line profiles in both cases were then presented and discussed.

We wish to highlight that the published $P(E_{\text{des}})$ in Fig. 4 of ref. 1 was actually that for the p-ASW surface and not the aSiO$_2$ surface as implied by the figure caption. This clearly necessitates correction. Fig. 1 below presents the correct figure. On further review of the work, we found that an early version of the $P(E_{\text{des}})$ curve for CO on aSiO$_2$ had been used to derive Fig. 5A and B and to populate Table 2. Fig. 2A and B and Table 1 present the corrected figures and table.

For ballistic deposition of CO on the aSiO$_2$ surface, there is no impact at all on the outcome of our simulations. Ballistic deposition cannot explain the line profile observed (Fig. 2A). In the case of the adsorb and diffuse mechanism, the corrected $P(E_{\text{des}})$ distribution produces a somewhat better fit (Fig. 2B) and at a slightly smaller linewidth than reported in our paper. This has the effect of further emphasising the linewidth difference between the C=O vibration on aSiO$_2$ and on p-ASW in a manner consistent with our argument that the presence of the underlying pseudo-continuous absorption due to the water libration + bend

Institute of Chemical Sciences, Heriot-Watt University, Edinburgh, EH14 4AS, UK. E-mail: m.r.s.mccoustra@hw.ac.uk

DOI: 10.1039/c9cp90226k
vibrational combination mode provides an additional pathway to relax the \( \text{C} = \text{O} \) vibration that reduces the lifetime and hence increases the linewidth on the p-ASW surface.

The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers.

References