

Surface specific adsorption of glucose to ZnO

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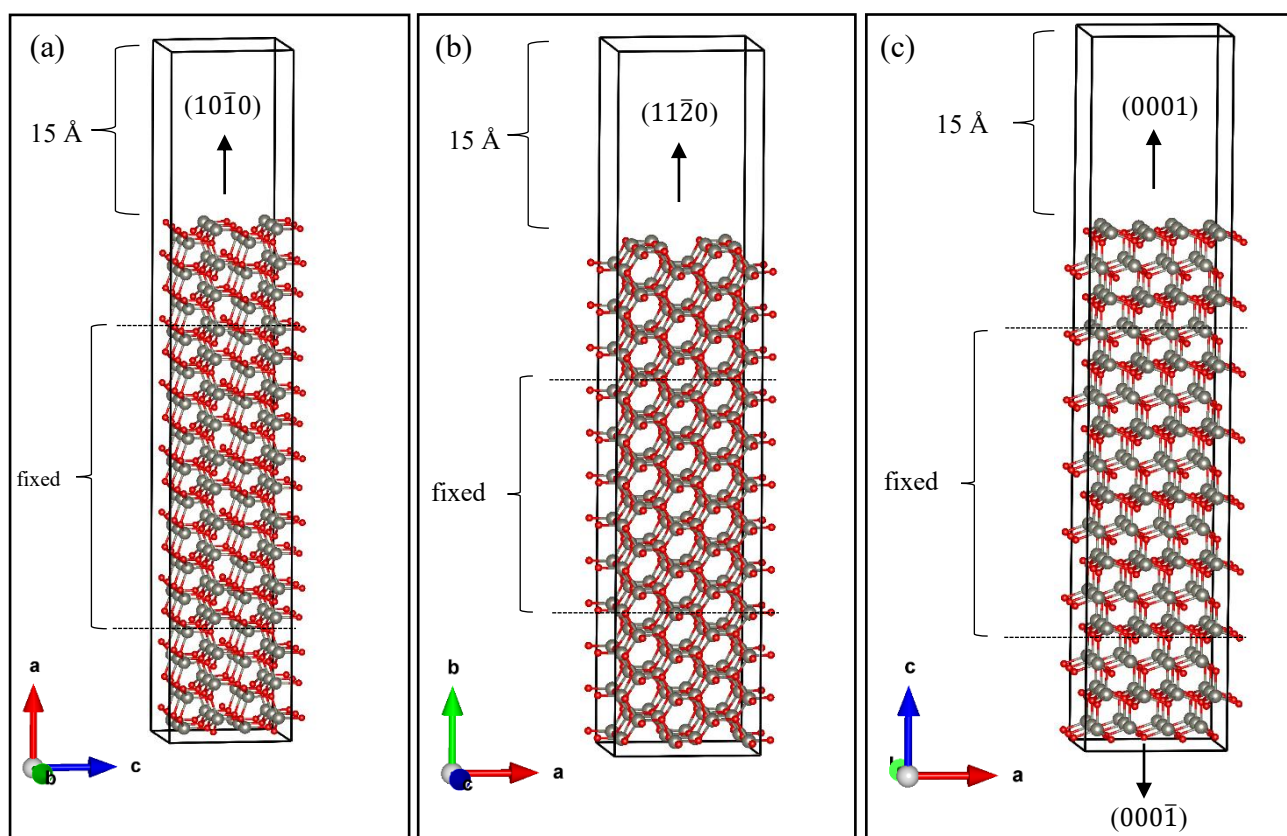


Fig. S1. Initial geometries of (a) $(10\bar{1}0)$, (b) $(11\bar{2}0)$ and (c) (0001) and $(000\bar{1})$ surfaces. For all the slabs, the first six layers on both sides are relaxed in all directions, while the other layers in the middle are fixed, shown in dotted lines. A vacuum of 15 Å is included above the surfaces.

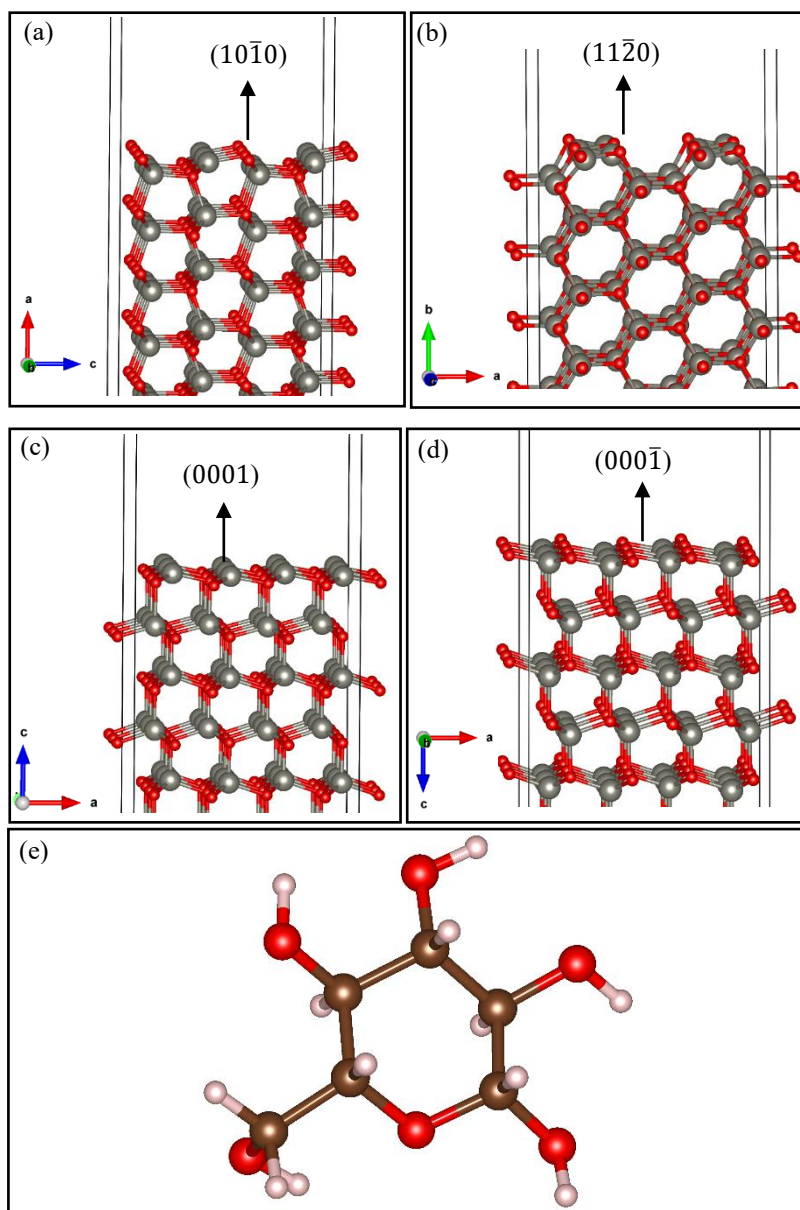


Fig. S2. Optimized geometries of (a) $(10\bar{1}0)$, (b) $(11\bar{2}0)$, (c) (0001) , (d) $(000\bar{1})$ surfaces and (e) glucose.

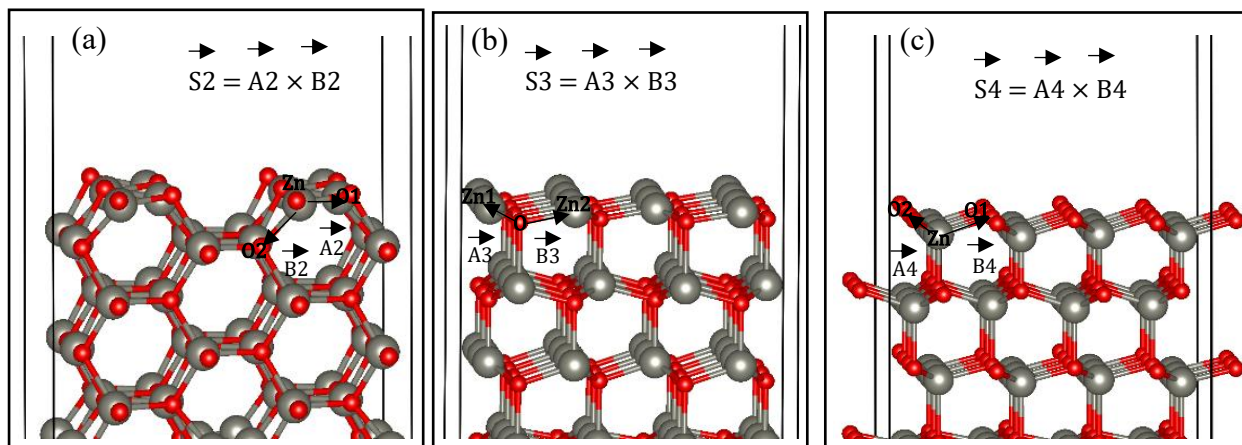


Fig. S3. Definitions of surface vectors for (a) $(11\bar{2}0)$, (b) (0001) , and (c) $(000\bar{1})$ surfaces.

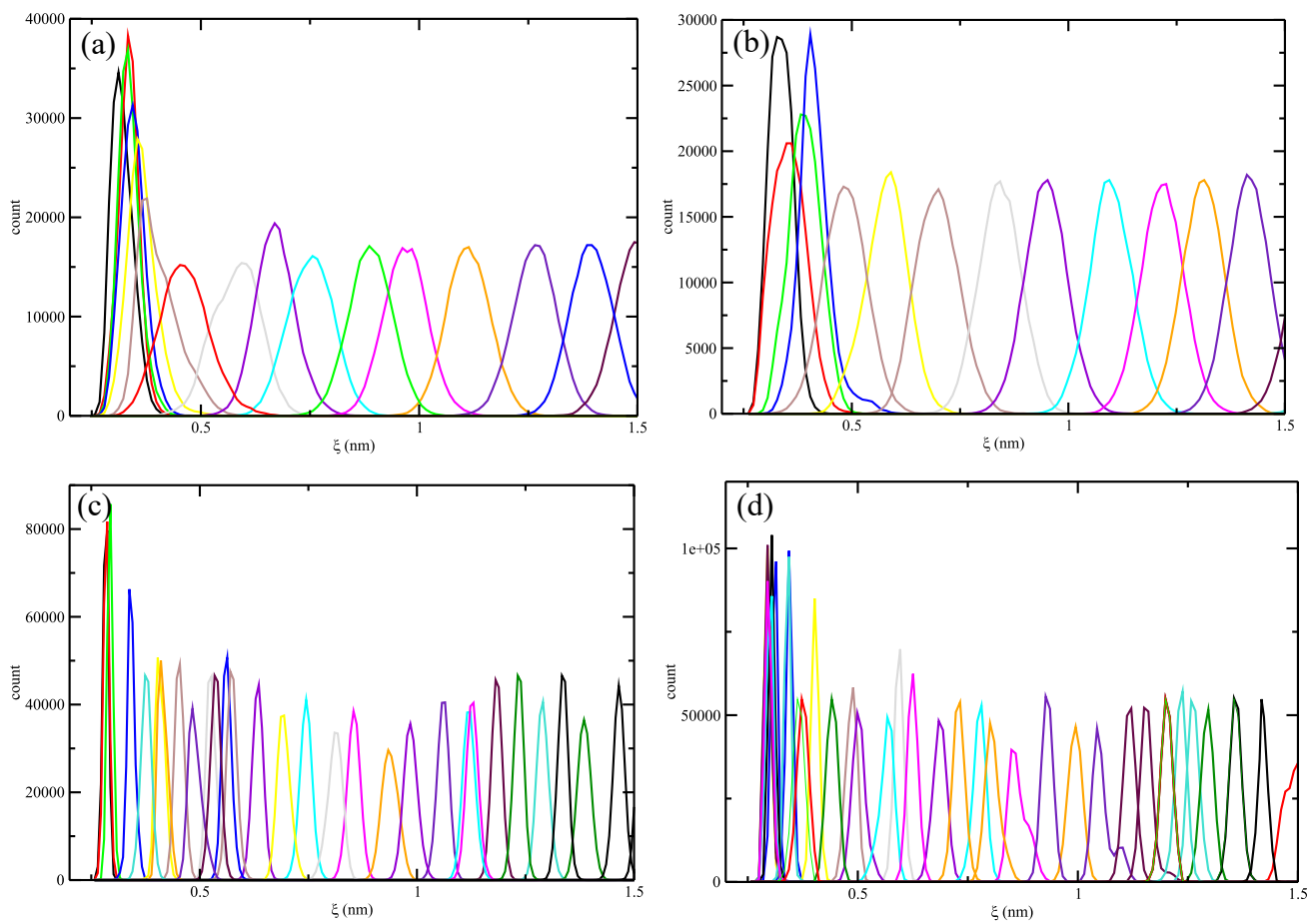


Fig. S4. Umbrella histograms for (a) $(10\bar{1}0)$, (b) $(11\bar{2}0)$, (c) (0001) , and (d) $(000\bar{1})$ surfaces.

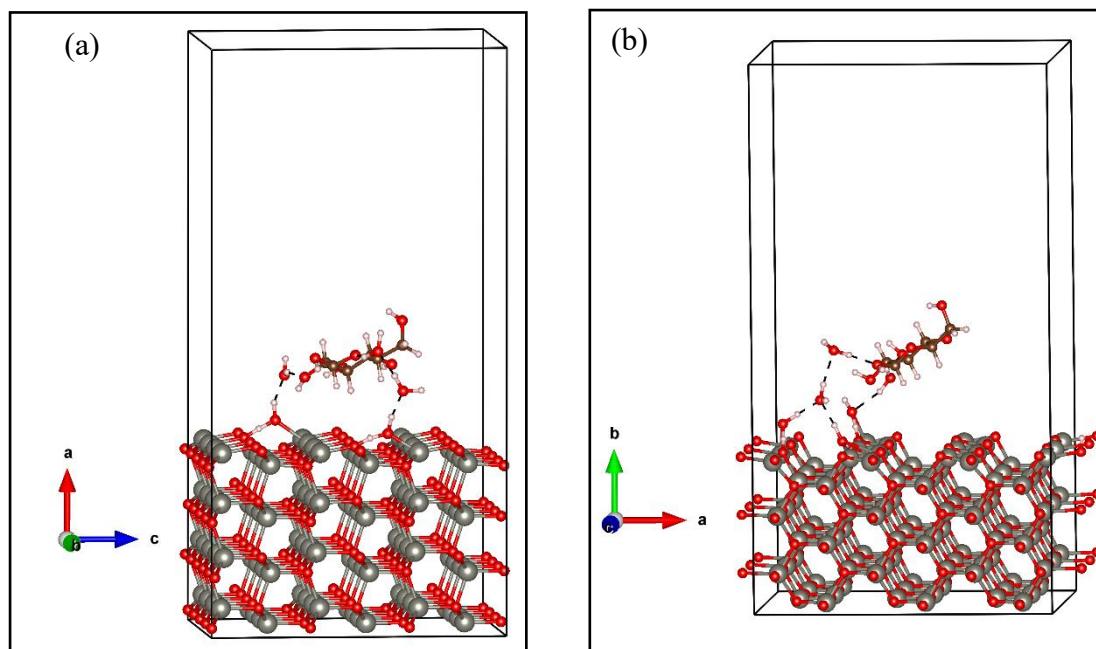


Fig. S5. MD snapshots of interactions between glucose and the surface via water molecules for (a) $(10\bar{1}0)$ and (b) $(11\bar{2}0)$ surfaces used for QM calculations.