Supporting Information: Molecular-level insight into ciprofloxacin adsorption on goethite: I. Approach and non-specific binding

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S1 Figures

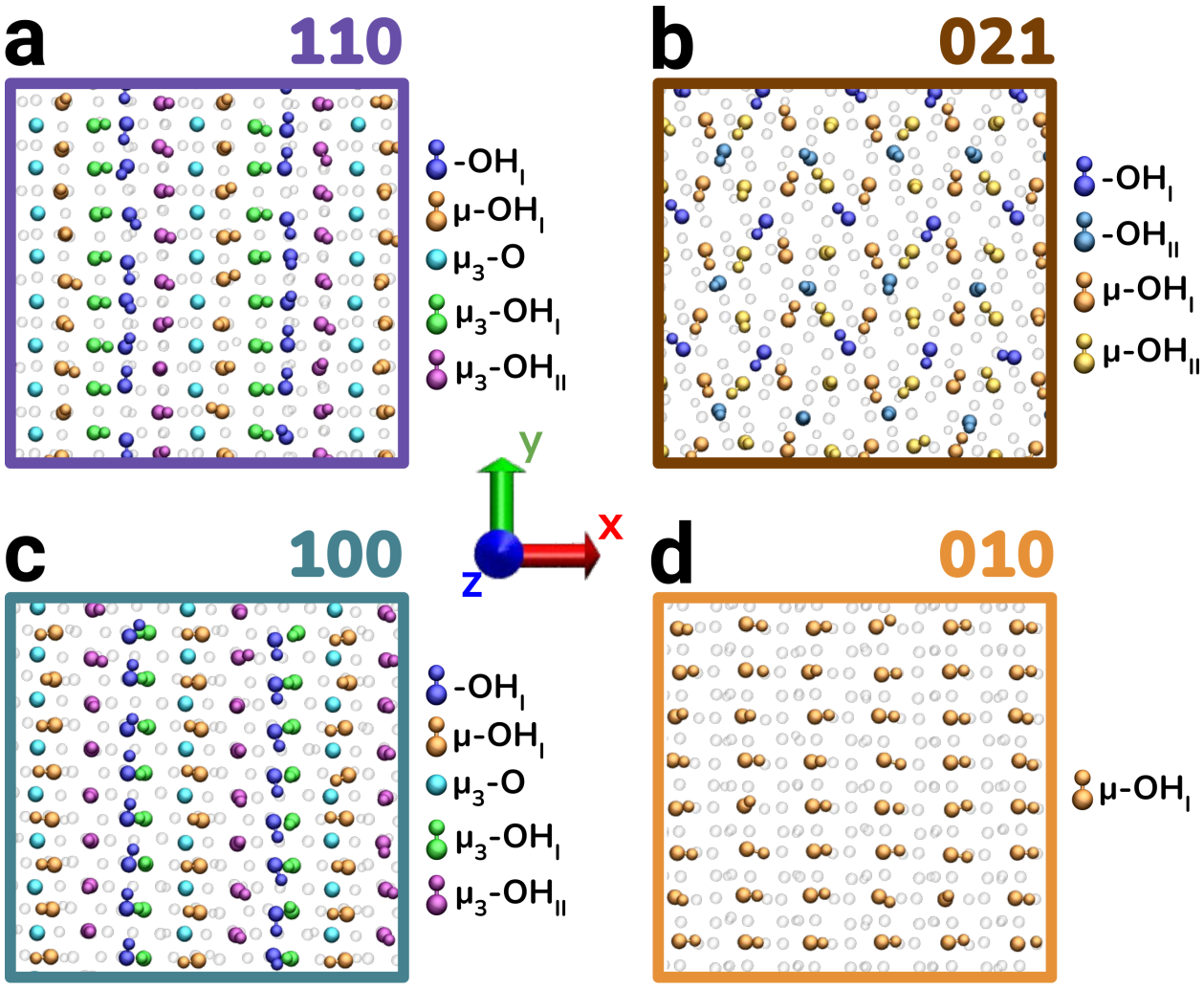

Figure S1: Snapshots with a top view of the four main crystallographic surfaces of a goethite (GT) particle, annotated with different surface groups/atoms: (a) 110, (b) 021, (c) 100, and (d) 010.

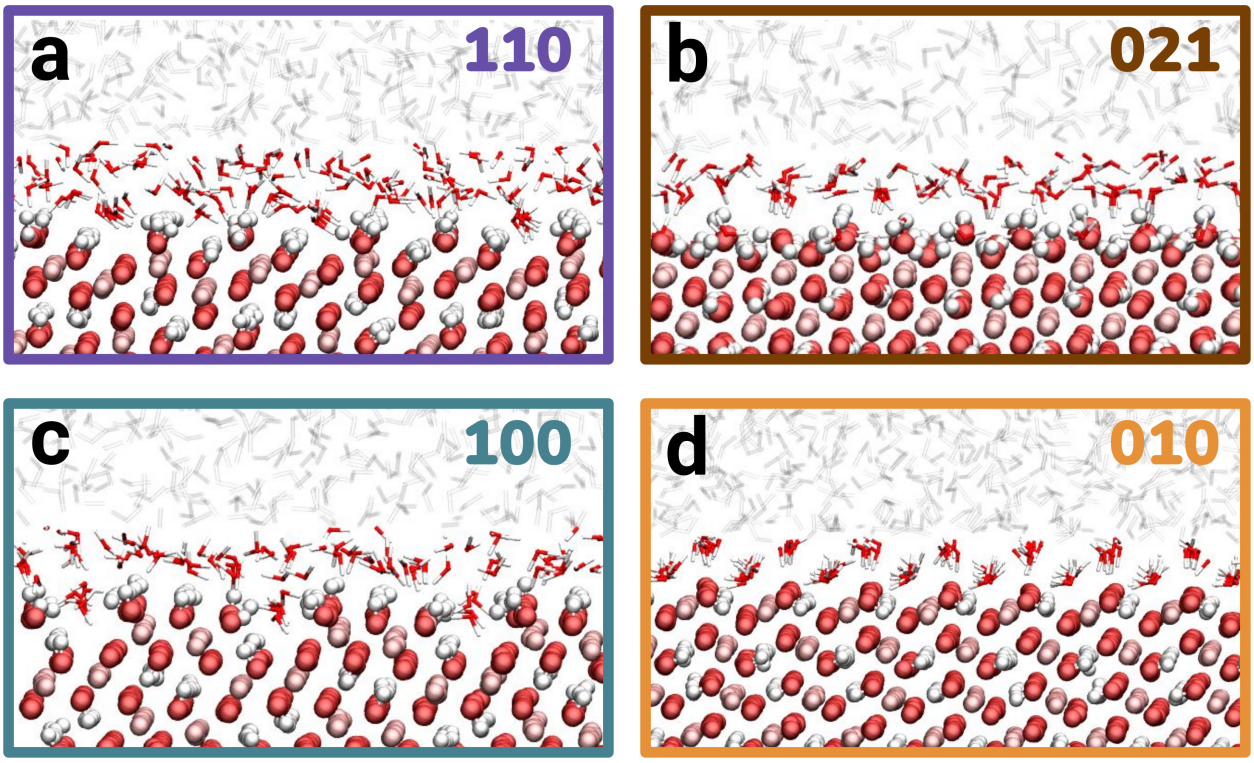

Figure S2: Snapshots focusing on the first two water layers on the GT surface (Figure 2) for the four crystallographic surfaces: (a) 110, (b) 021, (c) 100, and (d) 010.

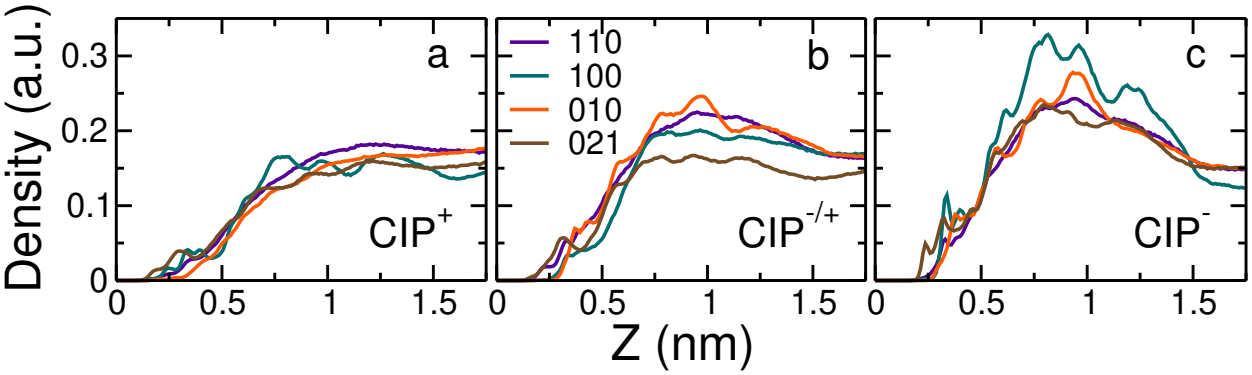

Figure S3: CIP molecules density profiles along the normal direction to the GT surface (Z) as a function of the GT crystallographic surface in contact with the solution for (a) CIP^{+}, (b) $CIP^{-/+}$, and (c) CIP^{-}.

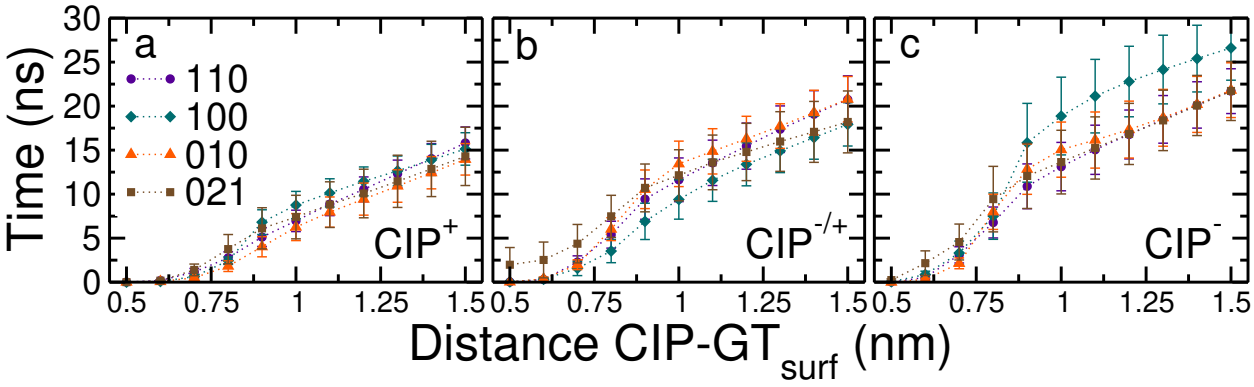

Figure S4: Average residence time of CIP molecules over a 50 ns simulation as a function of the distance from the GT surface for (a) CIP^{+}, (b) $CIP^{-/+}$, and (c) CIP^{-}. Error bars were obtained from the standard error over the ten simulations.

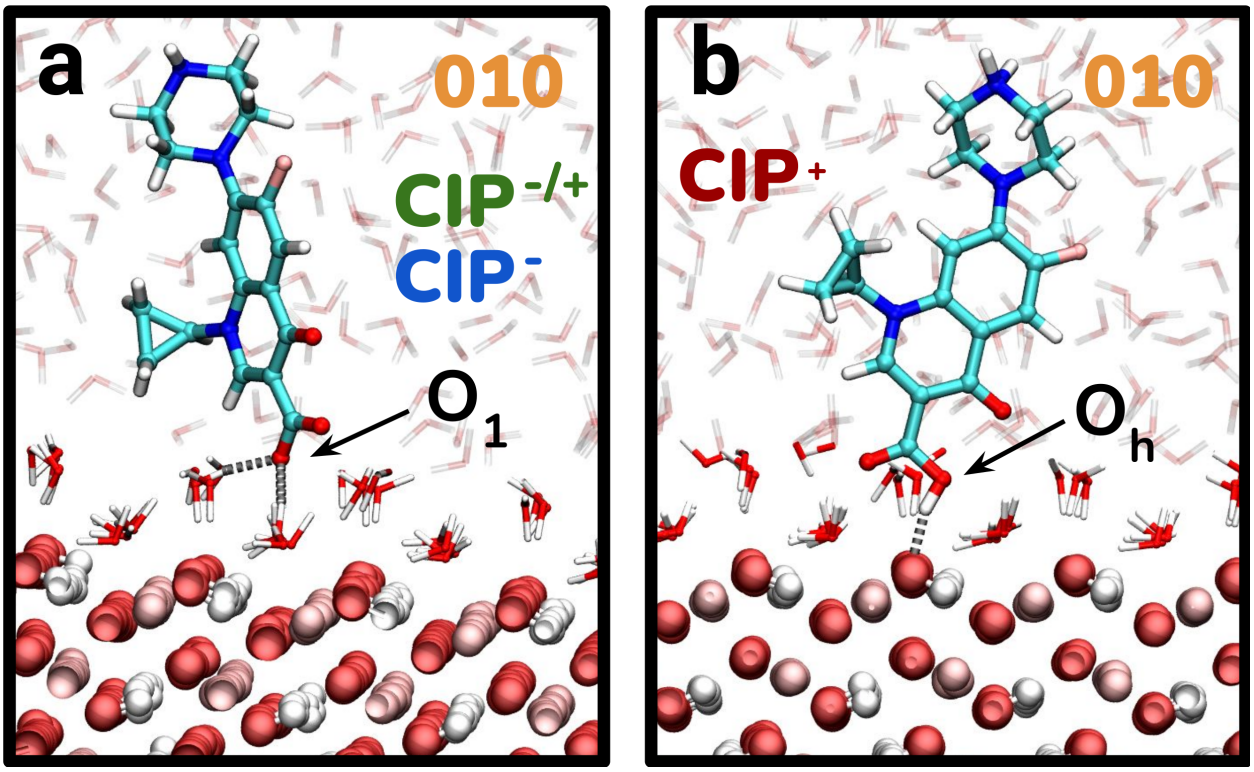

Figure S5: Snapshots of typical adsorption configurations of CIP molecules on the 010 GT crystallographic surface for (a) $CIP^{-/+}$ and CIP^{-}, (b) CIP^{+}. Gray dashed lines represent HBs between CIP molecules and GT surface/H_2O molecules adsorbed on the GT surface.

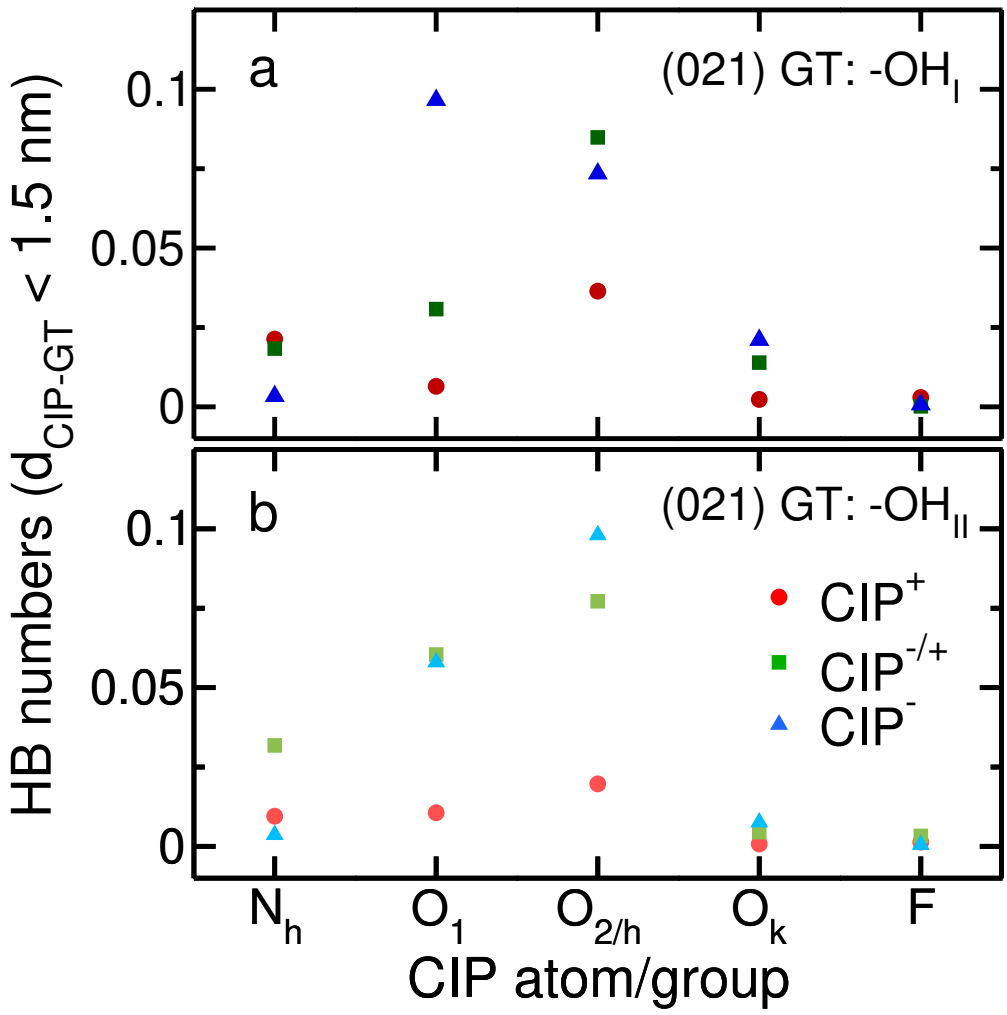

Figure S6: Average HB numbers per frame formed between CIP molecules and singly coordinated -OH groups of the (021) GT crystallographic surface when the distance between CIP molecules and the GT surface is less than 1.5 nm. HBs are represented according to the different atoms of the functional groups of the CIP molecules for singly coordinated OH group type: (a) OH_I and (b) OH_{II}.

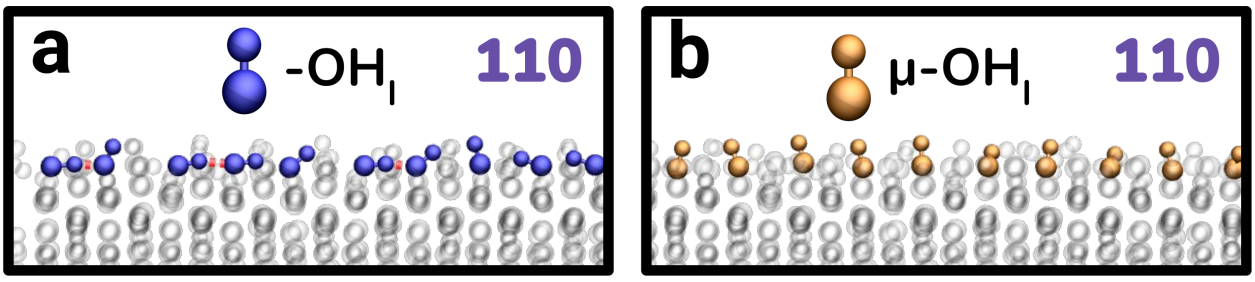

Figure S7: Snapshots of the 110 GT crystallographic surface focusing on surface hydroxyl groups: (a) singly coordinated OH_I and (b) doubly coordinated $\mu-OH_I$. Red dashed lines represent HBs formed between different OH_I groups within the same surface row.

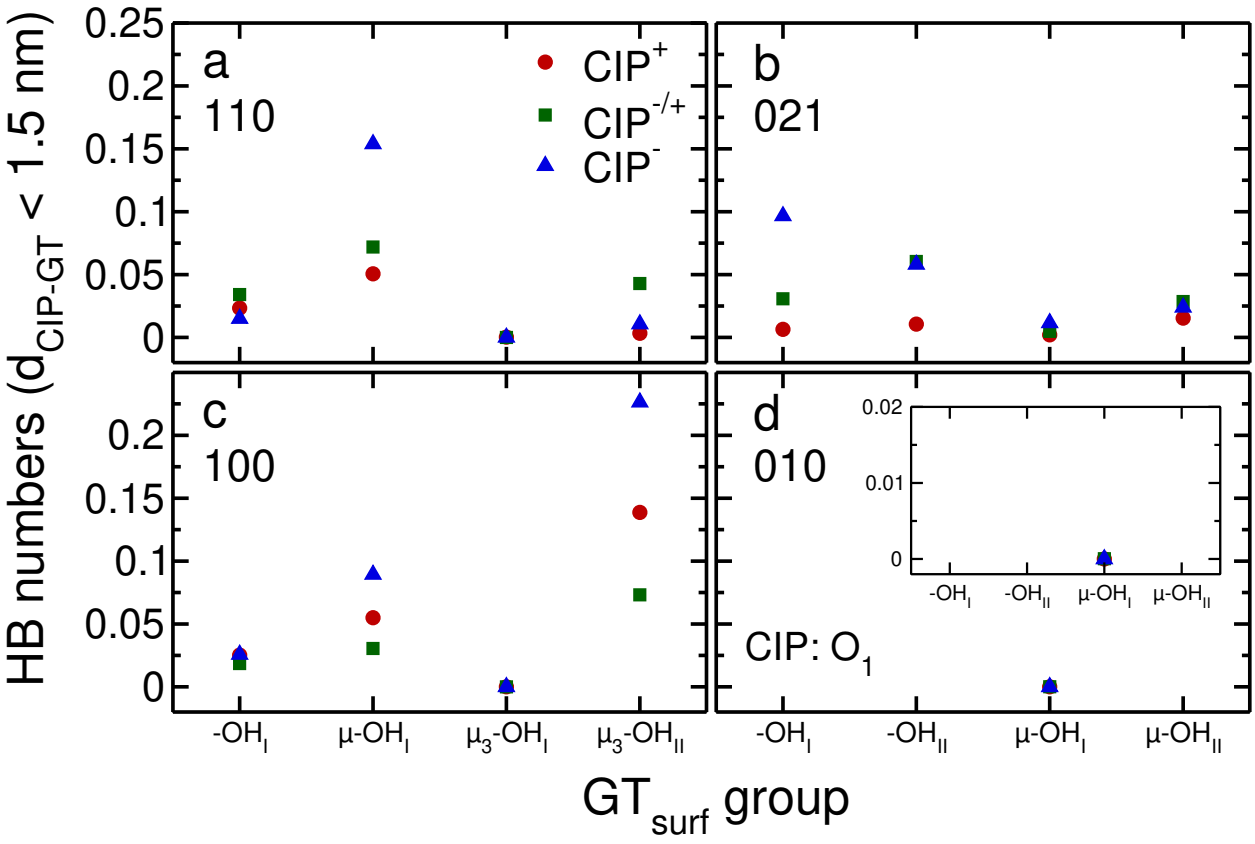

Figure S8: Average HB numbers per frame formed between the carboxylic acid oxygen atom O_1 and the GT surface when the distance between CIP molecules and the GT surface is less than 1.5 nm. HBs are represented according to the different atoms/groups of the GT surfaces for the four crystallographic surfaces: (a) 110, (b) 021, (c) 100, and (d) 010. The inset in panel (d) is a zoomed-in view of the graph in panel (d).

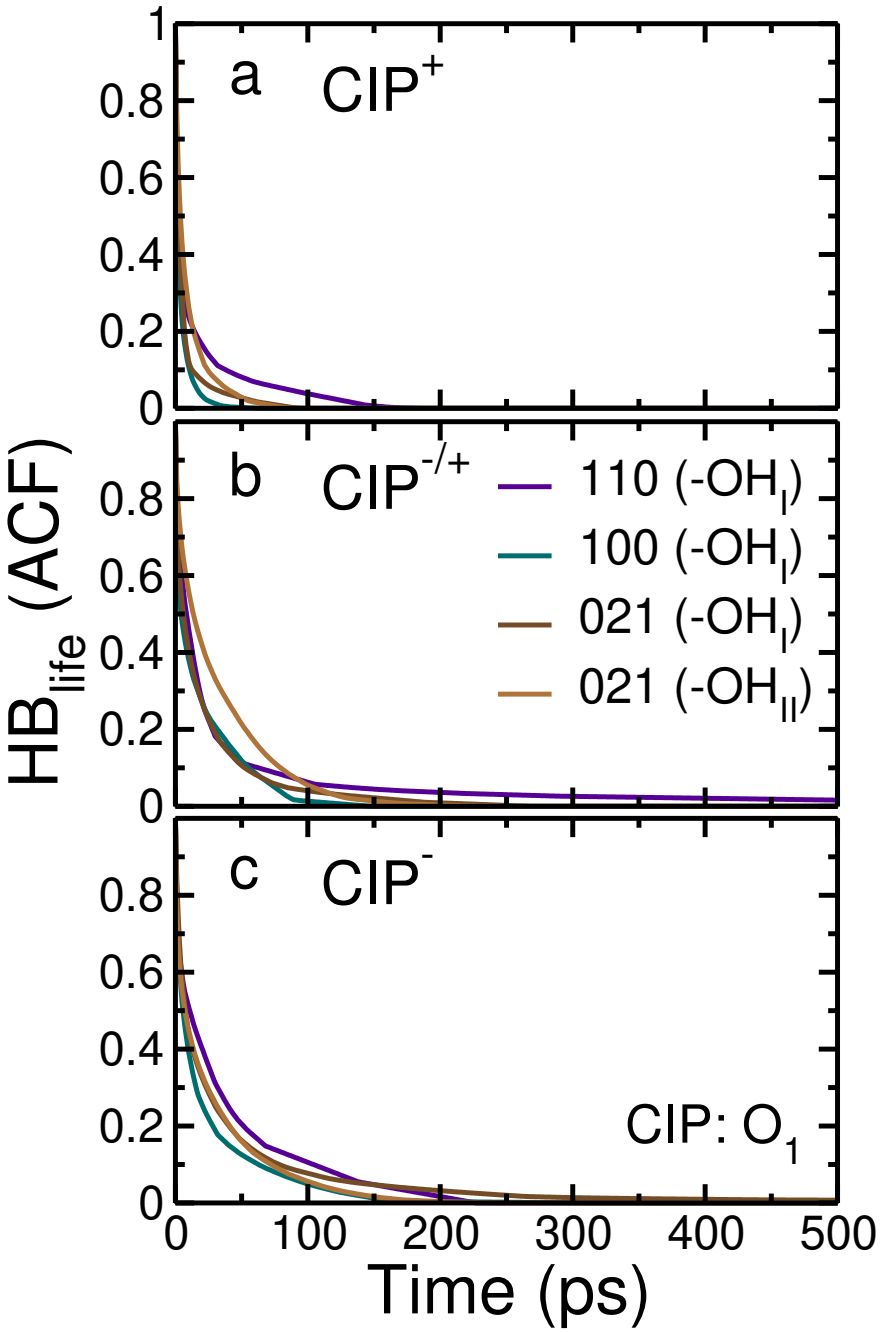

Figure S9: HB survival probability, measured by the autocorrelation function (ACF), formed between the carboxylic acid oxygen atom O_1 and the various singly coordinated hydroxyl groups on the four GT crystallographic surfaces for (a) CIP^+, (b) $CIP^{-/+}$, and (c) CIP^-.

Acknowledgement

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