Uptake and hydration of sulfur dioxide on the dry and wet hydroxylate silica surface: a computational study

Supporting Information

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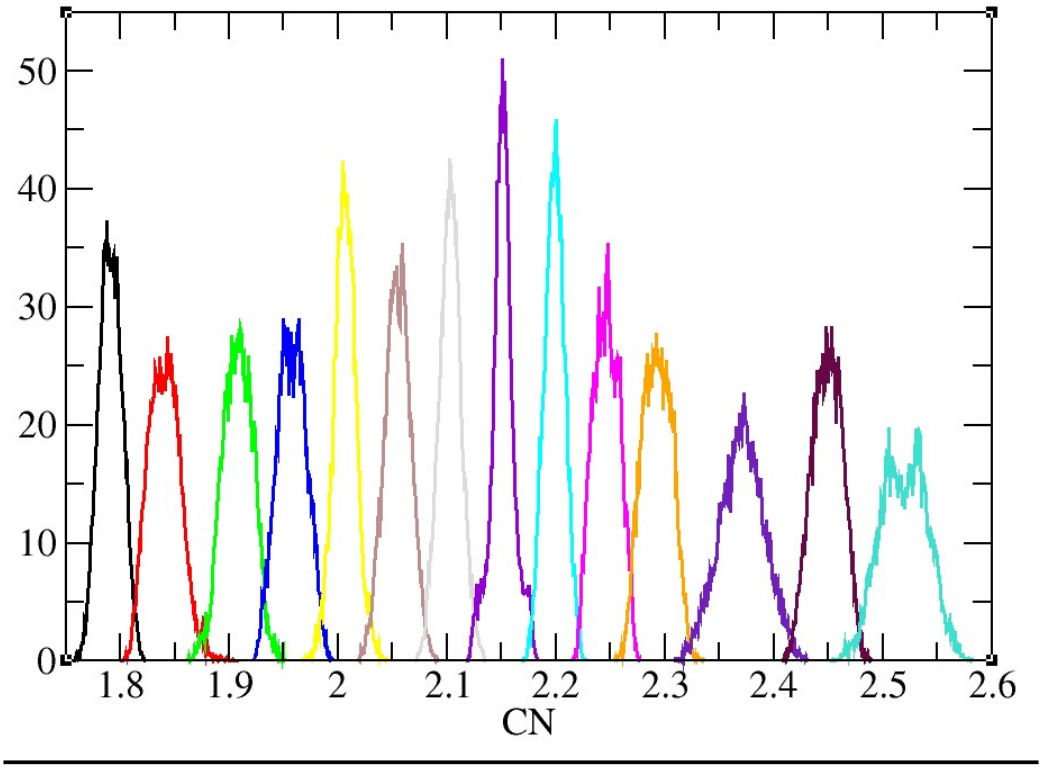

Figure S1: *Probability distribution for the CN reaction coordinate. Different colors represent the different umbrella runs used for the free energy profile calculation of SO_2 hydration on the dry surface. The first 2 ps of the*

umbrella trajectory were discarded for equilibration purposes.

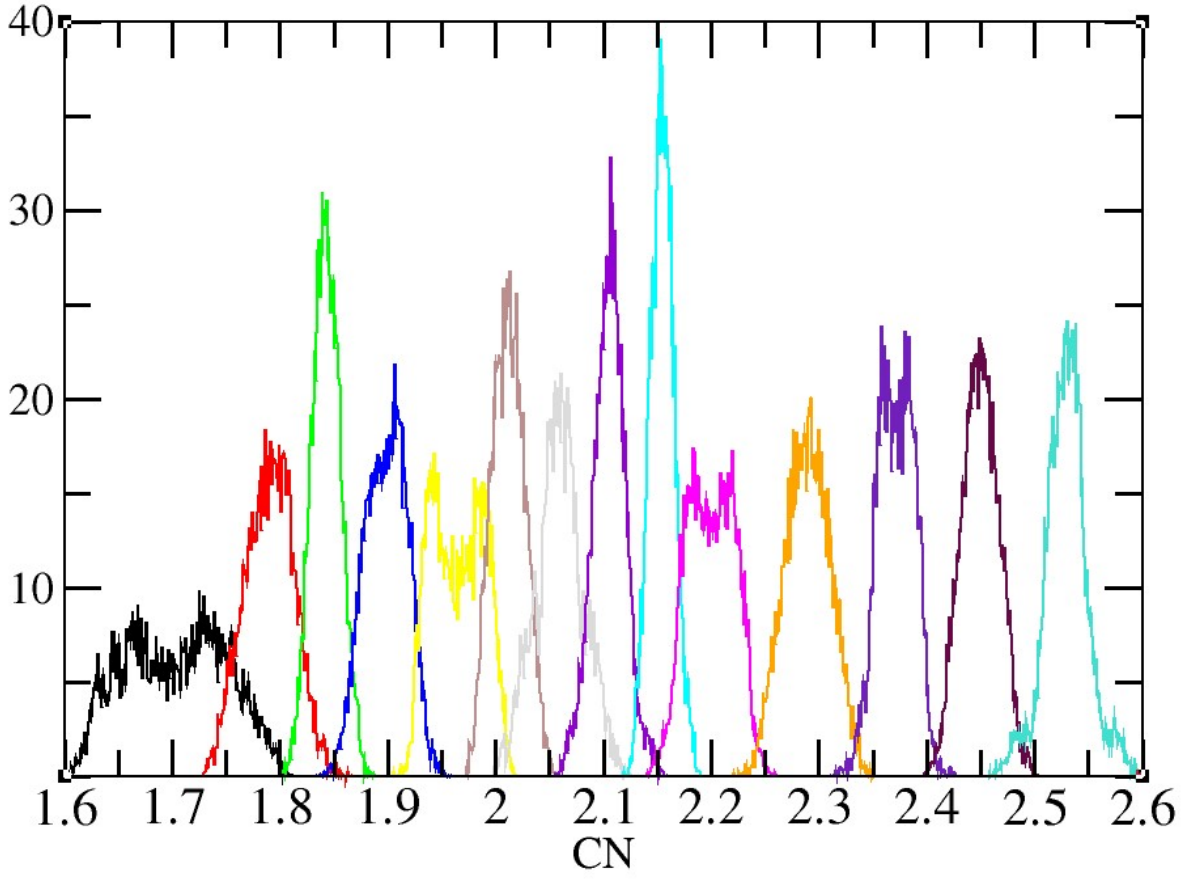

Figure S2: *Probability distribution for the CN reaction coordinate. Different colors represent the different umbrella runs used for the free energy profile calculation of SO_2 hydration on the wet surface. The first 2 ps of the umbrella trajectory were discarded for equilibration purposes.*

DRY	WET

CN	K(kJ/mol)	CN	K(kJ/mol)
		1.70	8000
1.8	16000	1.80	8000
1.85	16000	1.85	8000
1.90	16000	1.90	8000
1.95	16000	1.95	8000
2.00	16000	2.00	8000
2.05	16000	2.05	8000
2.10	16000	2.10	8000
2.15	16000	2.15	8000
2.20	16000	2.20	8000
2.30	16000	2.30	8000
2.40	8000	2.40	8000
2.50	8000	2.50	8000
2.60	8000	2.60	8000

Table S1: *The different CN values and spring constants used for the umbrella windows on the dry and wet surface.*