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Erratum

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Correction to An Explicit Consideration of Desolvation is Critical to Binding Free Energy Calculations of Charged Molecules at Ionic Surfaces

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We have recently noted an error in the unit conversion for Lennard-Jones parameters used for Ti and O atoms in TiO_2 in ref 1, the original paper. The correct parameters are summarized below in Table 1. Accordingly, the definition of the solvent coordination number variable (s) has been modified, that is, d_0 in eq 10 of ref 1 has been changed from 0.50 to 0.90. Using these parameters, we have recomputed the one-dimensional and two-dimensional potentials of mean force (PMFs), which are shown in Figures 1 and 2. The quantitative results differ from those presented in ref 1 (Figures 3 and 4); for example, the doubly bound (DB) state is now less stable than the singly bound (SB) state by a few kcal/mol, and the barriers that separate different states (DB, SB, and UB) are notably lower. However, the key observation remains the same; that is, the dominant barrier height from the 1D-PMFs is substantially different from the 2D result (by ∼6 kcal/mol), highlighting the importance of explicitly considering desolvation to binding free energy calculations. Therefore, the main conclusions from ref 1 remain valid.

Table 1. Lennard-Jones Parameters[2] for Ti and O Atoms in Rutile TiO_2

atom	q (e)	σ (Å)	ϵ (kcal/mol)
Ti	1.6910	0.7827	0.3355
O	−0.8455	1.6154	0.4573

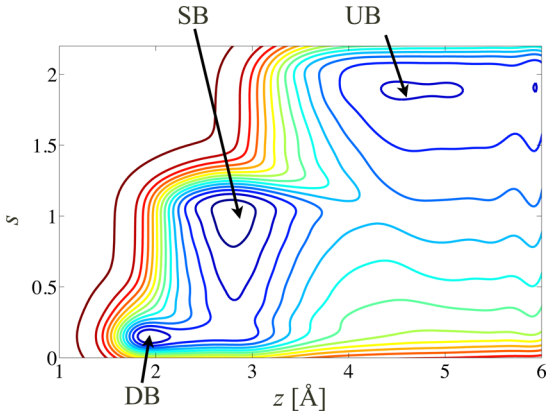

Figure 1. Two dimensional potential of mean force constructed from the two-dimensional metadynamics simulation. Contour line is drawn every 5 kcal/mol. DB, SB, and UB represent the doubly bound, singly bound, and unbound minima, respectively. Compare to Figure 3 of ref 1.

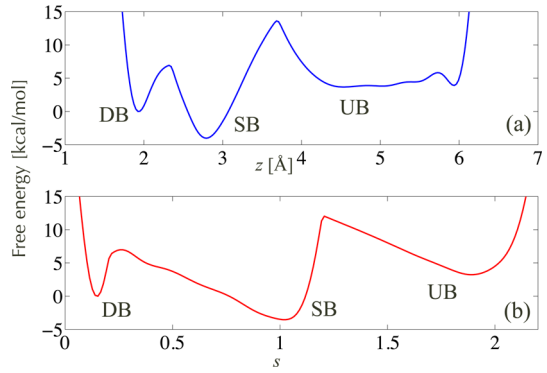

Figure 2. One dimensional potentials of mean force along (a) z and (b) s coordinates, constructed from the two-dimensional PMF in Figure 1 by integrating over the other coordinate. Compare to Figure 4 of ref 1.

REFERENCES

(1) Mori, T.; Hamers, R. J.; Pedersen, J. A.; Cui, Q. An Explicit Consideration of Desolvation is Critical to Binding Free Energy Calculations of Charged Molecules at Ionic Surfaces. *J. Chem. Theory Comput.* **2013**, *9*, 5059−5069.

(2) Schneider, J.; Ciacchi, L. C. A Classical Potential to Model the Adsorption of Biological Molecules on Oxidized Titanium Surfaces. *J. Chem. Theory Comput.* **2011**, *7*, 473−484.

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