

Electronic Effects on the Surface Potential at the Vapor–Liquid Interface of Water [*J. Am. Chem. Soc.* **2008**, *130*, 16556–16561]. Shawn M. Kathmann,* I-Feng William Kuo, and Christopher J. Mundy

Page 16560. In Figures 4 and 5 we presented results for the electrostatic potential at the vapor–liquid interface of water computed using the Hartree potential output from CP2K. We would like to thank Ming-Hsun Ho (Chemistry Department, University of Pennsylvania) for pointing out that the release of the code that we used for the Hartree potential had been corrected in a more recent version of the code. As a consequence, the error resulted in a Hartree potential that was $-169.9235344 \text{ bohr}^{-3}$ too small when compared to that determined using the newer, corrected release. This large correction changes the surface potential χ from -18 meV to $+3.1 \text{ eV}$, and the maximum interfacial electric field from the tanh fit changes from $+8.9 \times 10^7$ to $-1.5 \times 10^{10} \text{ V/m}$. The tanh fit parameters are $c_1 = 1.52434$, $c_2 = -8.31828$, and $c_3 = 1.56409$. The new Figure 5 is presented below. Future work will focus on understanding the implications of this on the electrical properties of interfacial water.

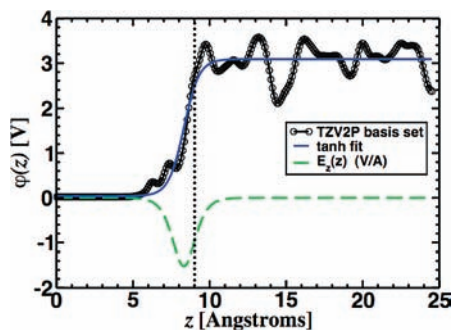


Figure 5. TZV2P data for the electrostatic potential $\varphi(z)$ (black circles) along with a tanh fit to the $\varphi(z)$ data (smooth solid blue curve) and the corresponding interfacial electric field $E_z(z)$ (dashed green curve). The Gibbs dividing surface (GDS) is located at $z = 9 \text{ \AA}$ (vertical dotted line).

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