Supplementary Information: Ion and Site Correlations of Charge Regulating Surfaces: A Simple and Accurate Theory

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Fig. S1 shows the effect of using $\zeta = 1$, including ion-ion correlation and ion-site correlations, on the titration behaviour as a function of $pH$ at various concentrations of (a) 1:1 salts and (b) 2:1 salts. There is a slight increase in surface charge density at the same conditions (i.e., salt concentration and $pH$), leading to a slightly worse agreement with the Monte Carlo results. However, the error is less than $\sim 5\%$, found at the highest $pH$ values, and given the approximative theory, this is still a tolerable error.

Fig. S2 shows the effect of having $\zeta = 1$ and $\xi^2 = 3$ for a couple of salts. While the 1000 mM 2:1 salt gives a good agreement with MC simulations (and experimental data), the agreement is only fair for 67 mM 2:1 salt and becomes worse for a 200 mM 1:1 salt.

Fig. S3 shows the effect of neglecting the $\phi^{ex}$ term, using $\zeta = 1$. All the curves show a weaker ionisation for the same salt, concentration, and $pH$. Lowering $\zeta$ or increasing $\xi^2$ will further decrease the ionisation, i.e., is not a viable approach.

Figure S1: (a) Same as Figure 2(d) but with $\zeta = 1$. (b) Same as Figure 3(d) but with $\zeta = 1$.

Figure S2: (a) Same as Fig. S1(a) but with $\xi^2 = 3$, (b) same as Fig. S1(b) but with $\xi^2 = 3$.

Figure S3: (a) Same as Fig. S1(a) but without $\phi^{ex}$, (b) same as Fig. S1(b) but without $\phi^{ex}$.