$x := 4$ $M := 25$ $L := x \cdot M$ $\alpha := 0.5$ $i := 1..1$

$Es := 0.3$ $Esw := 0.05$ $dE := 0.004$

$ne := 2$ $F := 96485$ $\Delta E := 0.6$ $R := 8.314$ $T := 298.15$

MATHCAD FILE for surface ECatalytic mechanism in DSWV

z = Kcat is dimensionless catalytic parameter
λ = KET is dimensionless parameter of electron transfer
Definitions and symbols of all other parameters are same as in the main manuscript file

$m := 1..\frac{\Delta E}{dE} \cdot L$ $step_m := Es - ceil\left(\frac{m}{L}\right) \cdot dE + dE$

$Eswf_m := if\left(L - 2M + ceil\left(\frac{m}{L}\right) \cdot L - L \le m \le L - M + ceil\left(\frac{m}{L}\right) \cdot L - L, Esw, 0\right)$

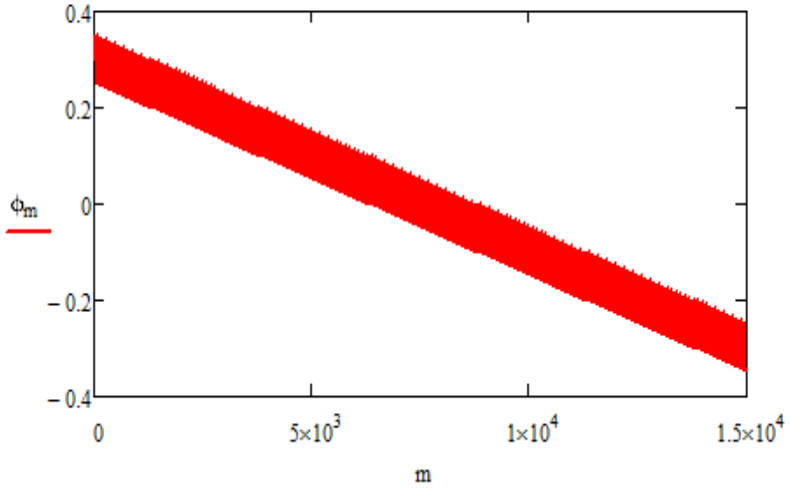
$Eswb_m := if\left(L - M + 1 + ceil\left(\frac{m}{L}\right) \cdot L - L \le m \le L + ceil\left(\frac{m}{L}\right) \cdot L - L, -Esw, 0\right)$

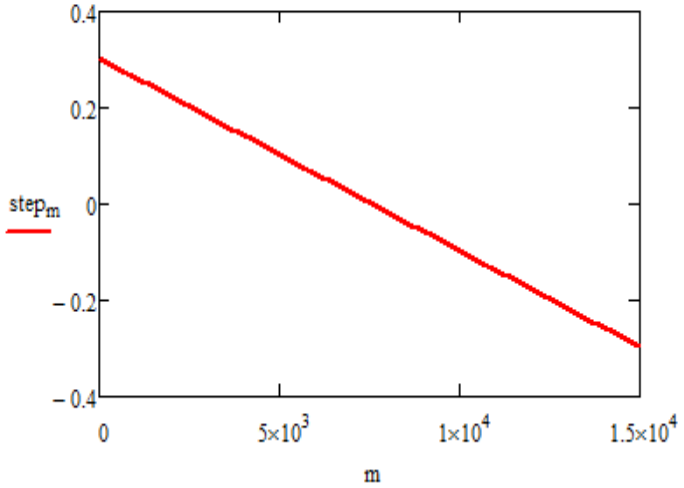
$\phi_m := step_m + Eswf_m + Eswb_m$ $\Phi_m := ne \cdot \frac{F}{R \cdot T} \cdot \phi_m$

Surface catalytic mechanism-theoretical study under conditions of differential square-wave voltammetry

Rubin Gulaboski, Valentin Mirceski

-Supplementary Material-





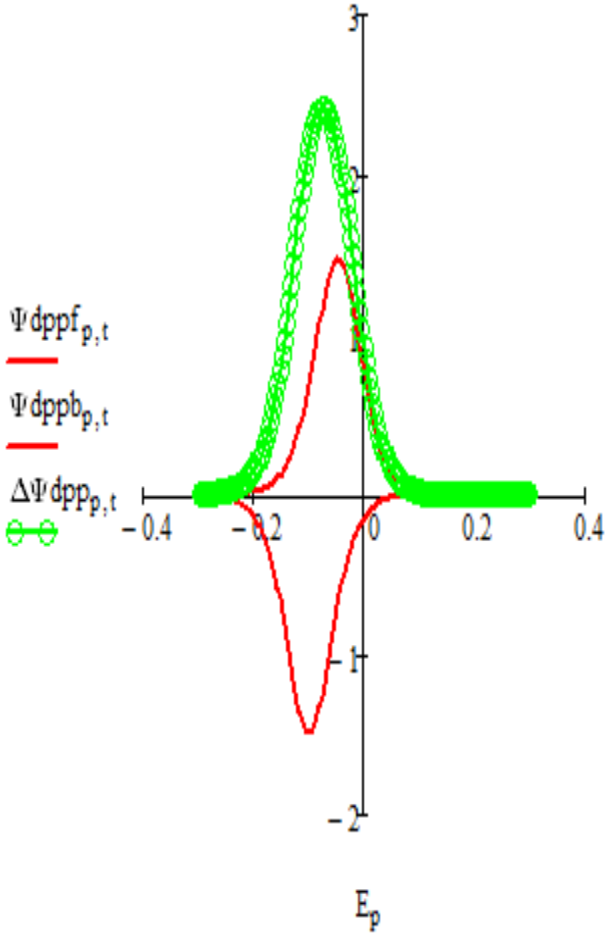
$\lambda_i := 0.18 \qquad z := 3.16 \qquad S_m := e^{\frac{-z}{50}\cdot(m-1)} - e^{\frac{z}{50}\cdot(-m)}$

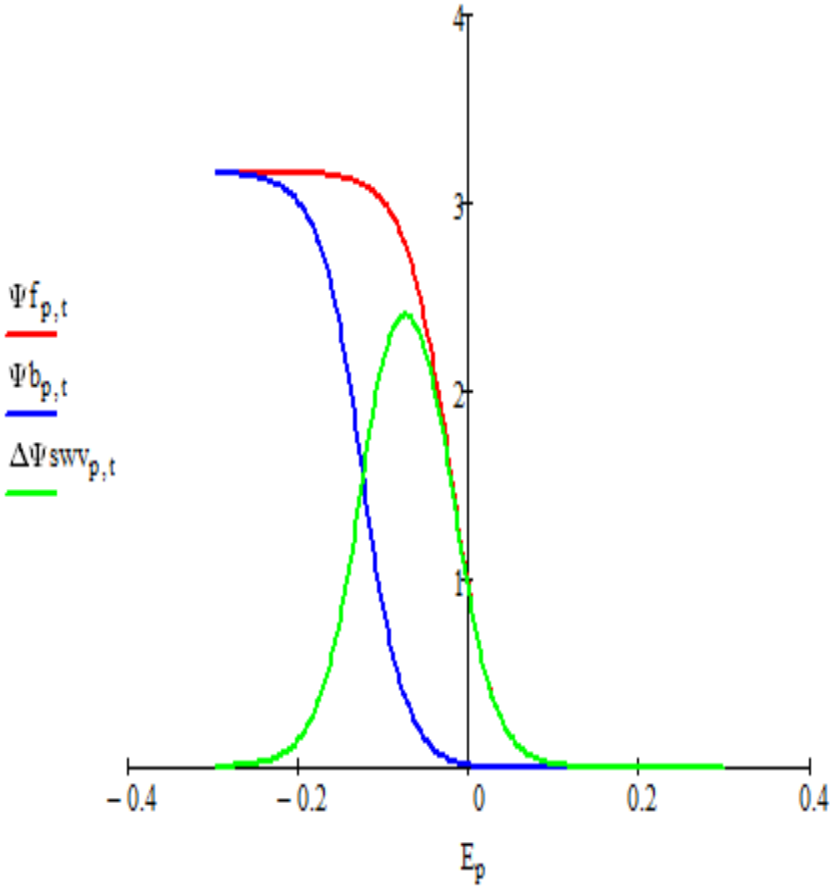
$$\Psi_{1,i} := \frac{\lambda_i \cdot e^{-\alpha\cdot\Phi_1}}{1 + \lambda_i \cdot e^{-\alpha\cdot\Phi_1}\cdot\left(1 + e^{\Phi_1}\right)\cdot\frac{S_1}{z}} \qquad \Psi_{m,i} := \frac{\lambda_i \cdot e^{-\alpha\cdot\Phi_m}\cdot\left[1 - \frac{1 + e^{\Phi_m}}{z}\cdot\sum_{j=1}^{m-1}\left(\Psi_{j,i}\cdot S_{m-j+1}\right)\right]}{1 + \lambda_i \cdot e^{-\alpha\cdot\Phi_m}\cdot\left(1 + e^{\Phi_m}\right)\cdot\frac{S_1}{z}}$$

$p := 1..\frac{\Delta E}{dE} \qquad E_p := (Es - p\cdot dE) + dE$

$\Psi base_{p,i} := \Psi_{p\cdot L-2\cdot M-1,i} \qquad \Psi b_{p,i} := \Psi_{p\cdot L-M,i} \qquad \Psi f_{p,i} := \Psi_{p\cdot L,i} \qquad \Delta\Psi swv_{p,i} := \Psi f_{p,i} - \Psi b_{p,i}$

$\Psi dppf_{p,i} := \Psi f_{p,i} - \Psi base_{p,i} \qquad \Psi dppb_{p,i} := \Psi b_{p,i} - \Psi base_{p,i} \qquad \Delta\Psi dpp_{p,i} := \Psi dppf_{p,i} - \Psi dppb_{p,i} \qquad \Delta\Psi_i := \max\left(\Delta\Psi swv^{\langle i\rangle}\right)$


Ψdppf p,t
Ψdppb p,t
ΔΨdpp p,t
3
2
1
−1
−2
−0.4
−0.2
0
0.2
0.4
Ep


Ψf p,t
Ψb p,t
ΔΨswv p,t
4
3
2
1
−0.4
−0.2
0
0.2
0.4
Ep