

2010, Volume 114C

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Modeling the Electrochemical Hydrogen Oxidation and Evolution Reactions on the Basis of Density Functional Theory Calculations

Page 18182. Equation 4 was realigned for clarity to the reader.

$$\begin{aligned}\Delta E_{\text{H}^*} &= E_{\text{diff}}(\theta_{\text{H}^*}) = \delta(N^*E_{\text{int}}(\theta_{\text{H}^*}))/\delta n \\ &= N^*\delta E_{\text{int}}(n/N)/\delta n \\ &= N(E_{\text{int}}(n/N) - E_{\text{int}}((n-1)/N))/\Delta n\end{aligned}\quad (4)$$

Equation 11 was corrected to the following:

$$r_{\text{T}}^{\text{HER}}(\theta) = \nu \sum_{i=0}^6 \binom{6}{i} \theta^{i+2} (1-\theta)^{6-i} \exp(-E_{a,i}^{\text{HER}}/k_{\text{B}}T) \quad (11)$$

Equation 12 was corrected to the following:

$$r_{\text{T}}^{\text{HOR}}(\theta) = \nu \exp(\Delta S/k_{\text{B}}) \sum_{i=0}^6 \binom{6}{i} \theta^i (1-\theta)^{8-i} \exp(-E_{a,i}^{\text{HOR}}/k_{\text{B}}T) \quad (12)$$

Various changes were made throughout the paper to correct or modify the text.

10.1021/jp110913n

Published on Web 11/29/2010