

For a heterogeneous electrode reaction, the current and overpotential are dependent of one another. (i) Write the equation that relates the current with overpotential. (ii) What is the name of this equation? (iii) For a heterogeneous electrocatalyst, the current can be activation controlled, mixed controlled, or mass transport controlled. Which current can be analysed by this equation? (iv) Can this equation be directly used to describe the current-over potential relationship of molecular electrocatalysis? Why or why not?

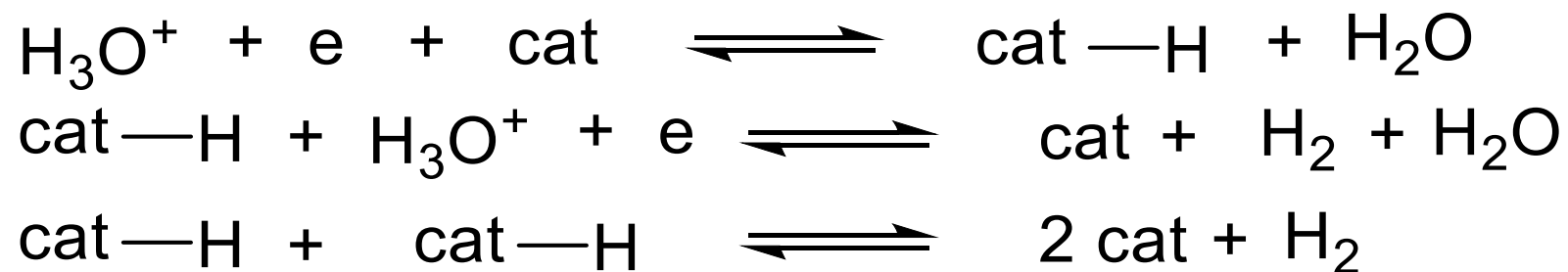
- $\eta = a + b \log I$ or something similar
- Tafel equation
- Only activation control current can be analyzed by the Tafel equation
- No, it cannot be used for molecular electrocatalysis because molecular electrocatalysis is easily influenced by diffusion of catalyst to electrode, so the current-over potential does not follow Tafel relation (or something similar; 1 point)

1. Two parameters can be obtained in a Tafel equation: exchange current and Tafel slope. Exchange current is a measure of “intrinsic activity” whereas Tafel slope describes how the current varies with the application of overpotentials. A catalyst has been improved by increasing the number of its active sites. Explain how this improvement affects the exchange current and Tafel slopes.

Increasing the number of the active site increase the exchange current, but does not change the tafel slope.

Many new hydrogen evolution catalysts in acidic solutions based on MoS_2 , Mo_2C and Ni_2P have been developed in recent years. To explain their high activity, people calculate the absorption energy of hydrogen atom on these catalysts. (a) Use the mechanism of hydrogen evolution on a heterogeneous catalyst to explain why hydrogen absorption energy is related to the HER catalysis. (b) Propose two methods how you can improve the HER activity of these materials.

The hydrogen absorption energy mimics the energy required for the first step, the formation of the M-H intermediate. If the M-H bond energy is too strong, it is hard for M-H to react further to make H₂. If the M-H energy is too weak, then the first step, the formation of M-H is difficult. Therefore, a good HER catalyst should have a modest M-H energy.



Strategies to improve the HER of materials:

1. Make small nanoparticles to have higher surface area; 2. Couple with a conductive substrate; 3. Use template to make materials with high active sites.