

Hydration Thermodynamics of ORR on Pt (111) : Comparison of Implicit and Explicit Solvation Models

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Nowadays, many groups devote themselves to find the optimal catalysts and it can help find the high-performance-materials in ORR. However, the insight of the interface between electrode and the electrolyte is lacked. Even though Pt has been studied for long periods and widely used, it has been still hidden. The solvation effect is highly related to the interface and many methods have been developed to contain this effect in thermodynamics of ORR. However, they failed to predict the actual onset potential. So, new method is needed to study the interface of the surface during the ORR and solvation effects should be studied. Here, we used grid-based explicit solvent method to consider the solvation effects during the ORR. Because it can describe the hydrogen bonds, impossible in implicit, it can predict the onset potential close to the experimental values than the implicit ones do. Interestingly the trend is similar in this method. Then, we find *O on the surface can make the reaction sluggish which can be the contradiction of common thoughts. And we concluded that *O₂ or *OOH dissociation to *O make the system worse.