DFT calculation for OH group around Pd on S-modified Au(111)

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Transition metal catalyzed reactions have played an important role in synthetic and process chemistry. The homogeneous catalyst surely causes effective reaction; however, a lot of efforts and energy are required for reusing the catalyst. From this viewpoint, development of the easily treatable heterogeneous catalyst is strongly desired for reducing the waste of expensive rare metal. Although the polymer supported catalyst has been developed, it cannot tolerate under severe conditions such as high temperature and it is restricted to use in organic solvents. On the other hand, Pd acetate (Pd(OAc)2) molecules immobilized on the S-terminated GaAs(001) has high catalytic activity and stability for Heck reaction [1]. However, the GaAs substrates including toxic As, it is not suitable for mass productions. To solve this problem, a new type catalyst was reported recently [2], which transition metals were supported on the S-modified Au(111). In order to develop more effective catalysts, it is essential to understand the function of the Pd catalyst of the S-modified Au(111).

Therefore, in this study, we tried to find the stable structure of Pd catalyst on the S-modified Au(111) by DFT calculations using the program package VASP [3].

The S atom is easier to be desorbed from the Au(111) substrate than the Pd atom during catalyst reaction. The binding energy of Pd atom is stronger due to the co-adsorption of S, the role of S is to make the binding of Pd stronger. We found that the stable position of Pd is lower place than S. We compared Pd on S-supported Au(111) with Pd on S-terminated GaAs(001)/GaN(0001), then we found that this kind of catalyst have a lot in common. [4,5]

References

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