Short Communication

A DFT Study on Application of Dual-Atom Fe₂/Phthalocyanine Catalyst for N₂ Reduction Reaction

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As the fundamental reactions, artificial ammonia synthesis via nitrogen reduction reaction (NRR) under mild environment is indispensable but challenging. In order to replace the commercial Ru catalyst, the development of the efficient catalyst with the abundant resource is of prominent significance. By density functional theory calculations, the NRR feasibility of dual transition metal doped phthalocyanine is systematically investigated wherein the Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn and Mo are considered as the dopants. The results reveal that the activity is highly sensitive to the TM introduction wherein the phthalocyanine with Fe₂ dual-atom center encounters the minimal thermodynamic barrier with the value of 0.19 V. Furthermore, the strong binding strength between the Fe₂ and its surrounding enables the excellent stability against clustering. In addition, the inverted-volcano curve is established between the thermodynamic barrier and the adsorption energy of *NNH, due to the difficulty of the first protonation. From the Mulliken charge analysis, the electron transfer between Pc and the adsorbents is occurred through Fe₂N₆ moiety. Overall, this work opens up the design of the robust electrode material for N₂-to-NH₃ conversion.

Keywords: nitrogen fixation, dual-site catalysts, density functional theory

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