

Computational Evidence for Hydrogen Generation by Reductive Cleavage of Water and α -H Abstraction on a Molybdenum Complex

Jun Li

State Key Laboratory of Materials-Oriented Chemical Engineering, Nanjing 210009

E-mail: lijun@njut.edu.cn

Abstract

Long-standing hypothesis now verified: H₂ generation by reductive cleavage of water and α -H abstraction has long been considered as a possible mechanism for reduction of water to H₂, but a clear example was not established up to now. Our detailed DFT calculations, based on the related experimental facts, now reveal that this process is energetically favorable on an Mo^I site (see Figure 1).

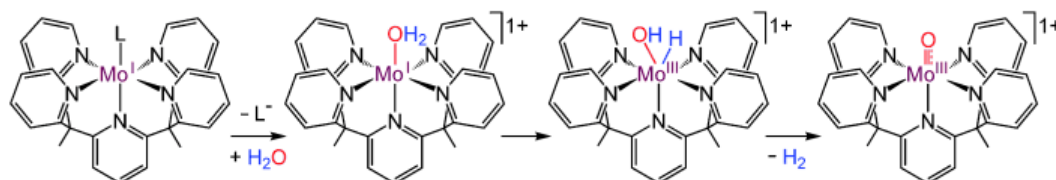


Figure 1. Reductive cleavage of H₂O and subsequent α -H abstraction on an Mo^I site.

Keywords:

Density functional calculations; Hydrogen generation; Water reduction; Molybdenum; Reaction mechanism.

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