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Water Adsorption and Dissociation on CeO₂(111). YI GAO, ZHONG-KANG HAN, Shanghai Institute of Applied Physics, Chinese Academy of Sciences, NAN SHAO, WAI-NING MEI, University of Nebraska-Omaha — The complexity and flexibility of ceria surface hinders the fully understanding of its reactivity and real applications. Here, we use H₂O/CeO₂(111) as the model system to investigate the water effect on the electron localization and vacancy diffusion on CeO₂(111) surface by the first-principle calculations. Our results indicate the water adsorption would high affect the electronic structures of CeO₂(111) surface, which further induce the dissociation of H₂O molecule. This molecular mechanism might provide more guidance to the future applications including the watergas shift reactions.

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