THE REACTION OF NANOSCALE ZERO-VALENT IRON WITH WATER

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Abstract
We present a combined theoretical and experimental study to decipher mechanism and kinetics of the reaction of water with nanoscale zero-valent iron in anaerobic conditions. The experimentally determined activation barrier corresponds reasonably well with the calculated barrier from the high level quantum chemical methods, which include dynamic electron correlation, relativistic effects and are crosschecked with different experimental thermochemistry measurements. The computations demonstrate two-step reaction involving two one-electron transfer processes and identify the rate limiting step. The implications for degradation of chlorinated hydrocarbons derived from the reaction mechanism and kinetics and nature of the reaction products are discussed.

Keywords: zero-valent iron, nZVI, water, reactivity, kinetics

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