

反应堆工程

压水堆核电站铁水反应机理研究

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收稿日期 修回日期 网络版发布日期:

摘要 从微观上研究压水堆核电站严重事故下减少或控制氢气生成的措施需研究氢气生成的微观机理。本工作采用量子化学理论, 应用量子化学软件包Gaussian03, 在B3LYP/6-311+G(d)理论模型上研究了压水堆严重事故下铁水反应的微观机理, 并计算了活化能。结果表明, 铁水反应是由两个基元反应组成的总包反应。第2步基元反应的正反应活化能较大, 是铁水反应的速控步。在微观上研究减少或控制氢气生成的措施应从第2步基元反应入手。

关键词 [压水堆](#) [铁水反应](#) [反应机理](#)

分类号

Study on Reaction Mechanism of Iron With Water in Pressurized Water Reactor

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Abstract The reaction mechanisms on hydrogen generation are the base of studying the microscopic measure to reduce or control hydrogen generation in the severe accidents for the pressurized water reactor plants. The quantum chemistry software Gaussian03 was used to study the reaction mechanism of iron with water at the B3LYP/6-311+G(d) theory model of quantum chemistry. The active energy was calculated. The results show that the reaction of iron with water is a total reaction, dividing into two elementary reactions. The reaction rate of the total reaction is determined by the second elementary reaction because of its higher active energy. It is concluded that the second elementary reaction should be the key elementary reaction to reduce the hydrogen generation.

Key words

[pressurized water reactor](#) [reaction of iron with water](#) [reaction mechanism](#)

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