

Joint CQSE and CASTS Seminar

Weekly Seminar
Mar. 2, 2012 (Friday)

TIME Mar. 2, 14:30 ~ 15:30
TITLE Spectroscopic Fingerprint of Water Decomposition:
ab initio Molecular Dynamic Study
SPEAKER Prof. Ming-Kang Tsai
Department of Chemistry, National Taiwan Normal University
PLACE Rm716, CCMS & New Physics Building, NTU

Abstract

Water radiolysis has been actively studied for over several decades due to its importance in nuclear reactor, storage of nuclear waste, industrial processes, and radiological therapy. OH radical is considered to be the predominant product by decomposing water. The quantitative characterization of OH radical generation and its subsequent reaction in aqueous environment plays an important role in controlling the safety of these intense chemical processes. The decomposition scheme water can be simply classified as three channels, i.e. cationic water, energized natural water, and anionic water. The natural channel can be further characterized by producing $H_2 + O$, $2H + O$, or $H + OH$, respectively.¹ Subsequent chemical reactions can progress further until the desorption of stable gas molecules H_2 and O_2 being driven by those reactive radical species – dominantly by OH radicals. The spectroscopic signal generated by electronic excitations of OH radical influenced by the vicinity hydrogen-bond network is commonly used to monitor the reaction dynamics of water radiolytic processes, and to study the scientific fundamentals of these electron-initiated decomposition processes. In the present study, *ab initio* molecular dynamic simulations are used to investigate the neutral, cationic, and radical fragments of small water system. The dynamics of the corresponding excited states will also be characterized. The implication of decomposing water cluster based upon these calculations will be discussed.

Reference:

- (1). B. C. Garrett et al., Chem. Rev. 2005, 105, 355-389.

