

Abstract Submitted
for the NEF16 Meeting of
The American Physical Society

Study on Organic Wastewater Contaminants(OWCs) Using Computational Simulation and Chemical Physics DAHYUNG KIM, ANDREW KYUNG, Choice Research Group — Amongst the global water crisis, the conservation of fresh water supply on Earth is crucial. Industrialization and the resulting pollution have posed a serious threat to our water sources. Synthetic chemicals used in manufacture and industry are often wrongfully disposed and contaminate the water supply. Some of the synthetic chemicals, categorized as organic wastewater contaminants (OWCs), include pharmaceuticals and hormones. Chemical compounds in such substances can cause various health defects in living organisms, such as cancer, abnormal reproductive function, change in physiological processes, and development of antibiotic resistance. However, the low concentrations of pharmaceuticals, hormones, and personal care products(PPCPs) present in industrial runoffs make it difficult to observe its resulting health defects. In this paper, theoretical and computational calculations, through computational chemistry and program package, used the restricted approximation of the wave functions to calculate the safety and stability of the PPCPs. The Universal Force Field (UFF), a molecular mechanics force field theory was employed to predict the thermodynamic properties of the PPCPs molecules.

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Date submitted: 09 Oct 2016

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