

Abstract Submitted
for the TSF19 Meeting of
The American Physical Society

Study on the Effective Flavescens Molecules to Capture Fine Dust Using Chemical and Computational Analysis JIMIN BAEK, IOLANI School, SO MIN LEE, The Hun School — Various industrial pollutants, including heavy metals such as mercury and cadmium, have been major causes of health problems. The heavy metals are ubiquitous air pollutants which are increasing in the environment and they are responsible for many disease processes including carcinogenesis. These diseases are often attributed to poorly-detected air pollutants. Since there is a strong association between flavescens molecules and the effectiveness in fine dust removal, the effective flavescens molecules were modeled and analyzed using chemical and computational analysis. The molecules are also used in medical applications for their anti-inflammatory effects and effective activity in radical scavenging. The reactivity and conductivity were measured through the dipole moments to calculate the activity level the molecule could have with other nearby molecules. Also, electrostatic potential maps were utilized to visualize the polarization and assess the reactivity level of each molecule. The primary purpose of this research is to analyze the thermodynamical and stereochemical safety of several types of flavescens molecules and to find thermo-chemical properties of their derivatives that could be used as agents used in the air pollutants removal.

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Date submitted: 08 Oct 2019

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