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Study on Efficiency of Nanoparticles and Chelate Ions for Water Purification Using Chemical and Computational Analysis BRIAN KIM, RICHARD KYUNG, CRG-NJ — Increasing water pollution and lack of clean water all around the world is a rising global crisis. Recent studies have found several compelling methods of water purification: using metal oxide, carbon nanotube, metal-organic framework, Ethylenediaminetetraacetic acid, and diethylenetriaminepentaacetic acid. The purpose of this project is to study the potential use of these chemicals by testing their efficiency and effectiveness. The efficiency of these chemicals was measured by analyzing their optimization energy, dipole moment, and electrostatic map. The electrostatic map visualizes the charge distribution throughout the molecule, the dipole shows the charge difference within an unequally shared bond, and optimization energy shows the energy needed to optimize a molecule to its prime shape. For higher efficiency, colorful electrostatic maps, high dipole moment, and low optimization energy are needed. A computer program was used to measure the optimized geometries and chemical properties. The modeled structures and atomic properties were analyzed by using electron density theory and considering stereochemical effects of the molecules.

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