

Abstract Submitted
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Study on the Thermo-chemical Effects of the Nano Scaled Cosmetic Molecules Using Computational Analysis EMILY W. CHUNG, Global Christian Foreign School - GCFS, AMANDA KYUNG, NVRHS — Components in cosmetics or sunscreens can be degraded in the existence of UV light and the photodegradation causes a loss of UV protection irritating skin or damaging DNA in cells. In this research, computational methods employing quantum chemistry were used to model various components in sunscreens. The safety of the molecules were checked by assessing thermodynamic stability, reactivity and polarization. Thermodynamic stability was measured through the optimized energy and the reactivity and conductivity were measured through the dipole moments to calculate the level of activity the molecule could have with other nearby molecules. Lastly, electrostatic potential maps were also used to visualize the polarization and assess the reactivity level of each molecule. Molecules in the sunscreen with lower optimization energies were predicted to be more thermodynamically stable than those with higher optimization energies. Molecules with higher dipole moment were predicted to be more active than those with lower dipole moment. Also, molecules with more colorful electrostatic potential map was predicted to be more active than those with less colorful electrostatic potential map.

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