Biochemical Stability Analysis of Nano Scaled Contrast Agents Used in Biomolecular Imaging Detection of Tumor Cells JENNIFER KIM, RICHARD KYUNG, Choice Research Group — Imaging contrast agents are materials used to improve the visibility of internal body structures in the imaging process. Many agents that are used for contrast enhancement are now studied empirically and computationally by researchers. Among various imaging techniques, magnetic resonance imaging (MRI) has become a major diagnostic tool in many clinical specialties due to its non-invasive characteristic and its safeness in regards to ionizing radiation exposure. Recently, researchers have prepared aqueous fullerene nanoparticles using electrochemical methods. In this paper, computational simulations of thermodynamic stabilities of nano scaled contrast agents that can be used in biomolecular imaging detection of tumor cells are presented using nanomaterials such as fluorescent functionalized fullerenes. In addition, the stability and safety of different types of contrast agents composed of metal oxide a, b, and c are tested in the imaging process. Through analysis of the computational simulations, the stabilities of the contrast agents, determined by optimized energies of the conformations, are presented. The resulting numerical data are compared. In addition, Density Functional Theory (DFT) is used in order to model the electron properties of the compound.