Abstract Submitted for the MAS15 Meeting of The American Physical Society

Evaluation of the Biocompatibility of the Bioinert Zirconia Using Computational Simulation YEON TAE CHUNG, SAEGYUL RHEE, GUN HA SEO, Choice Research Group — One of the essential requirements of the biocompatible implants is restoring lost tissues. The choice of medical and dental implant materials is also important. To enhance the osseo-integration, researchers have been developing metal oxides, such as titanium oxides, as medical and dental implant materials. The improvements in new materials make it possible to have durable fixtures made of ceramic, which is commonly known as zirconia, a more tissue friendly material. Before fabricating a customized zirconia implant in a factory, it is recommended to test the stability of the molecular compound in order to verify its practical use. This paper shows how the zirconia implants perform better than the titanium oxide by employing computational chemistry methods. The commercial programs such as Gamess and Chemcraft have been used in an effort to discover the optimal method and to compute the measurements of stability. For the molecular diagrams, bond strengths are indicated by either a solid line or dotted line - greater the number, the stronger the bond. Any number greater than 1 is known to be very strong. If oxygen is not attached to the rest of the compound, it probably means the compound does not exist with oxygen.

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Date submitted: 02 Oct 2015

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