Abstract Submitted
for the MAS21 Meeting of
The American Physical Society

Study on the Nano-scaled Functionalized Biochemical Particles for the Treatment of Neurodegenerative Diseases EUNKI SHIM, Philips Academy Andover — Iron homeostasis is currently emerging as a key factor in maintaining brain health and preventing disease. In several common neurodegenerative diseases such as Alzheimers Disease (AD) and macular degeneration, dyshomeostasis of redox-active metals and subsequent detection of elevated levels of redox-active metals such as iron and copper in the brain suggests that such metals play a significant role in the pathogenesis of such disease. In this paper, computer programs were used to model various chelators that were potential candidates for iron chelation therapy in the brain. The molecules were assessed for thermodynamic stability, reactivity/conductivity, and polarization. Thermodynamic stability could be measured through optimized energy. Generally, as optimized energy decreased, thermodynamic stability increased. Reactivity/conductivity was measured through the dipole moments and may act as a good indicator of how the molecule may interact with surrounding particles in vivo. Lastly, electrostatic potential maps were used to visualize the polarization and assess the reactivity level of each molecule.

Richard Kyung
CRG-NJ

Date submitted: 05 Nov 2021 Electronic form version 1.4