

Abstract

Ultra-small, water-soluble, white light-emitting (WLE), highly stable (~8 months) BSA templated metallic (Mg^0) nanoclusters (fluorescent magnesium nanoclusters=FMNCs) are developed using the green and facile route. Synthesis was facilitated by the reduction of magnesium salt, where template bovine serum albumin is utilized as a reducing agent, and ascorbic acid acts as a capping agent to impart stability in water, thereby obtaining stabilized Mg^0 nanocluster. Several spectroscopic and microscopic techniques, such as UV-Vis spectroscopy, TEM, XRD, XPS, FTIR, confocal microscopy, MALDI-TOFF, and CD spectroscopy, confirmed the synthesis of metallic magnesium nanoclusters. In solution, stabilized Mg^0 nanoclusters produce white light (450-620 nm with FWHM~120 nm) upon 366 nm light excitation. This white light emission was found to have a CIE coordinate of 0.30, 0.33 [pure white light CIE (0.33, 0.33)]. Taking advantage of WLE and ultrasmall size, FMNCs were used for *in-vitro* fluorescence imaging of HaCaT cell lines, yielding blue ($\tau = 2.94$ ns, with a relative of QY= 1.2 % w.r.t QS), green ($\tau = 3.07$ ns; relative quantum yield of 4.6% w.r.t R6G) and red ($\tau = 0.3$ ns) images. Further, incubation of FMNCs with HEK293 (Human embryonic kidney cell) and cancerous MDA-MB-231 (Breast cancer cell line) human cell lines yielded 100 % cell viability. Current work is envisioned to contribute significantly in the areas of science, engineering, and nanomedicine. Afterward, Multifluorescent, water-soluble magnesium nanoclusters (lyz-MgNCs) were synthesized using positively charged protein lysozyme (lyz) and ascorbic acid as the reducing agent and capping agent, respectively; the as-prepared particles were 3-4 nm in size at neutral pH. They exhibited multifluorescent emission at 450, 545, and 628 nm when excited at 366, 469 and 560 nm wavelength, respectively, and exhibited a maximum quantum yield of 5% (Ex. 366) and 6.8 % (Ex. 469). Additionally, prepared clusters decorated with anomalous properties such as excellent photostability, good ionic strength tolerability, and broad-range pH stability. The Lyz-MgNCs prepared at neutral

pH show 95% cell viability in brain cell (UT-87 MG) lines and hence can be used as a probe for cellular imaging. Furthermore, the demonstration of imaging was carried out using glioma brain cell lines, viz., UT 87 MG cells, and revealed significant cytoplasmic accumulation in the red, green, and blue regions. The Z-stack study revealed the presence of Lyz-MgNCs in the depth of cells. Furthermore, in vivo toxicity assessments revealed the nontoxic behavior of the prepared particles, and real-time tracking through IVIS imaging in rodents confirmed their candidature for biological cell imaging/labeling purposes. In addition, to capitalize biocompatibility and angiogenic response of magnesium, we explored its antimicrobial efficacy to harvesting their role in wound care; in this regard, an essential oil-derived 37 nm-sized metallic magnesium-based gel (Magnogel) has been procured from one pot facile greener route. The prepared gel demonstrated excellent bactericidal activity against *E. coli* (ATCC 25922 strain), *S. aureus* (ATCC 29213 strain), and fungicidal effect against *Candida albicans* (ATCC 10231) strain. The lowest determined MIC values were as low as 0.017 $\mu\text{g}/\mu\text{l}$ for *E. coli* and 0.008 $\mu\text{g}/\mu\text{l}$ for *S. aureus* bacteria, whereas, for candida albicans fungi, the reported inhibitory concentration is 0.035 $\mu\text{g}/\mu\text{l}$. Moreover, toxicity assessment of prepared gel was driven on fertilized chicken egg using CAM assay revealing negligible toxicity and angiogenic response at MBC concentration of *E. coli* (0.03 $\mu\text{g} / \mu\text{l}$). Additionally, the Prepared gel was tested for pH and spreadability properties. However, visual inspection determined the organoleptic appearance (clarity, odor), grittiness, and gel homogeneity. Furthermore, understanding thermodynamic parameters, nucleation rate, and interfacial energy is crucial to predicting the prepared cluster's stability, size, and phase, and it could be tuned to acquire desirable properties. To understand the thermodynamic and kinetic properties of ultra-small magnesium prenucleation clusters, for computation of nucleation rate at high temperature ($>100^\circ\text{C}$), thermogravimetric analysis (TGA) was utilized for the first time. The exploration of temperature-dependent nucleation is required to appraise the extent of kinetic and

thermodynamic barriers associated with the origin of subatomic-size nuclei, which control the nucleation rate. The precise computation of nucleation rate, thermodynamic parameters, and interfacial surface energy for ultra-small clusters (0.5-2 nm) is still absent in the high-temperature range. Here, apparent activation energy (E_a), thermodynamic parameters (ΔG , ΔH , and ΔS), and pre-exponential kinetic factor were estimated by the utmost accurate Vyazovkin advanced and KAS iso-conversional techniques for calculation of nucleation rate and interfacial energy for ultra-small magnesium clusters ($\sim 0.8 \pm 0.24$ nm), in the temperature range from 555 to 780 K. The master plots propounded the existence of random nucleation in the magnesium metal matrix over a specified conversion. Based on the above findings, four mathematical models are proposed to compute nucleation rate and interfacial energy in magnesium clusters over respective temperatures and conversions. These models are beneficial for predicting the nucleation rate and interfacial energy over a high range of temperatures and specific conversion.