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MODELING OF STERIC HINDRANCE OF NANOPARTICLES

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The stability of nanoparticle dispersion plays an important role in many applications, such as printed electronics, electrowetting display. The current work studies the relationship between steric force due to the polymer-based capping molecules and the macroscopic properties in solutions. Based on the theory of Brownian dynamics, a computational model is developed to reveal the mechanism of the nanoparticle aggregation in solutions with and without the capping molecules. Suitable potentials related to the interaction of atoms and steric repulsion are found and implemented. In addition, the surface charge of the particles (zeta potential) and the properties of the solution are modeled. The effective radius of the clusters in the solution subject to different conditions are predicted and validated with the experimental data of particle size distribution generated by light scattering technique. The results are expected to provide guidelines for the design of capping molecules and the optimization of the synthesis procedures of nanoparticle solution.

REFERENCES

[1] K. J. Lee, B. H. Jun, T. H. Kim, and J. Joung, Direct synthesis and inkjetting of silver nanocrystals toward printed electronics, *Nanotechnology*, vol. bf 17, no. 9, pp. 24242428, May 2006.

[2] J. R. Spaeth, I. G. Kevrekidis, and A. Z. Panagiotopoulos, A comparison of implicit- and explicit-solvent simulations of self-assembly in block copolymer and solute systems, *The Journal of Chemical Physics*, vol. **134**, no. 16, pp. 16490216490213, Apr. 2011.

[3] Y. Hu, B. Wu, Z. Xu, Z. Yang, and X. Yang, Solvation structure and dynamics for passivated Au nanoparticle in supercritical CO2: A molecular dynamic simulation, *Journal of Colloid and Interface Science*, vol. **353**, no. 1, pp. 2229, Jan. 2011.