Brownian dynamics simulations of electrostatic adsorption and ordering of charged colloidal nanoparticles JENNIFER LUNA-SINGH, Rice University, US Air Force Research Laboratory, ENRIQUE BARRERA, Rice University, VIKAS VARSHNEY, Universal Technology Corporation, US Air Force Research Laboratory, JOHN KELLEY, UES, Inc., US Air Force Research Laboratory, RICHARD VAIA, US Air Force Research Laboratory — Self-limiting assembly of nanoparticle (NP) and biomacromolecular arrays promises to revolutionize compliant device fabrication by enabling print-on-demand. Presently, quantitative understanding of the relationship between the array order, nanoparticle size, surface characteristics, and process conditions remain elusive. Previous simulations have shown that tuning particle and surface potentials, screening lengths, and particle concentrations can lead to ordering. However, identifying the experimental conditions to observe these in-plane order-disorder and order-order transitions for NPs remains a challenge. Here in, the absorption of electrostatically stabilized NPs with increasing ratio of particle-particle repulsion to particle-surface attraction via Brownian dynamics simulations is discussed. The orientation correlation function follows the KTHNY theory of phase transition as particle and surface potentials are tuned. Detailed Voronoi analysis reveals movement and defect annihilation during the final stages of adsorption. Identifying the transition between liquid, hexatic, and crystalline NP arrays will provide experimental conditions necessary to create high resolution patterns and smaller devices.

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