## *IN SILICO* OPTIMIZATION OF 3D NANOSTRUCTURED PLASMONIC CRYSTALS

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We present two types of plasmonic crystals composed of metal coated, square arrays of either nanowell or nanopost structures formed via soft nanoimprinting as Surface Enhanced Raman Scattering (SERS) substrates. Such crystals exhibit SERS enhancement factors of $10^5$ to $10^6$, over large areas and with sufficiently high levels of uniformity for precise two-dimensional Raman mapping of surface bound monolayers. Three-dimensional finite-difference time-domain (3D FDTD) simulations qualitatively capture the key features of these systems and suggests a route to the fabrication of optimized, highly efficient SERS substrates *in silco*. Collectively, the ease of fabrication together with the high sensitivities and spatial resolution that can be achieved suggests an attractive route to the design and optimization SERS substrates for portable chemical warfare agent detection, environmental monitors, noninvasive imaging of biomolecules, and other applications.