Modeling Super Repellant Nanostructured Surfaces for Chemical Biological Defense

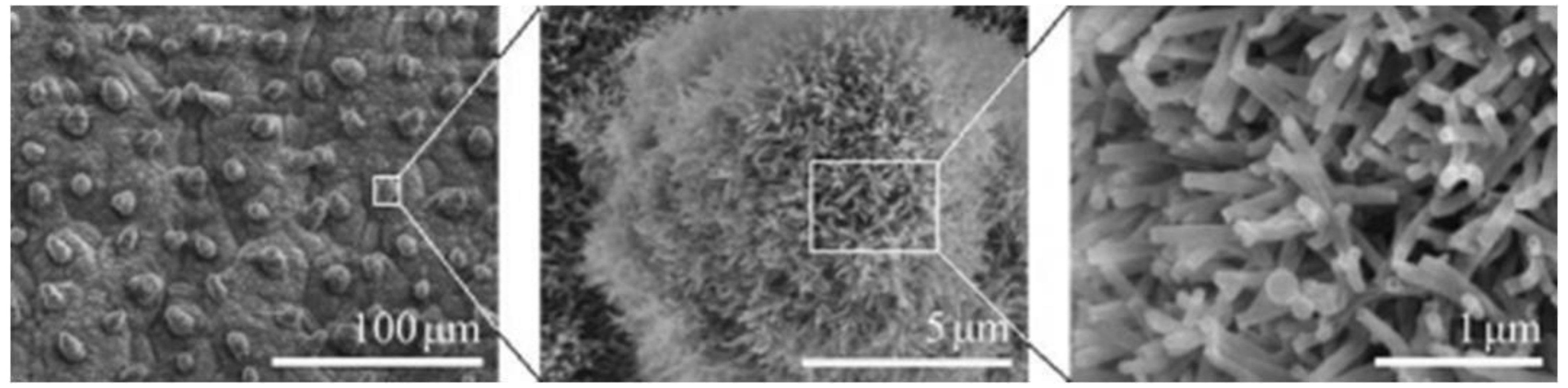
Craig K. Knox [1], Jerry B. Cabalo [2], Gary K. Kilper [3], Stephanie Ihejirika [2]
(1) Leidos, Inc., (2) U.S. Army Edgewood Chemical Biological Center, (3) Excet, Inc.

Abstract

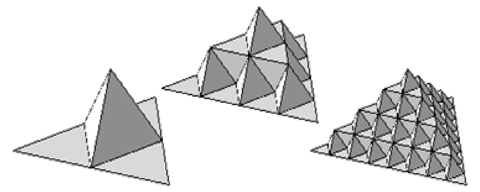
Contamination of surfaces by deposition of aerosol particles is a process that affects a broad array of application areas, including pharmaceutical and food production, as well as chemical and biological defense. The deposition of particles is driven by particle-surface adhesion. Using atomistic simulations, we examined the role of nanostructures in minimizing the interaction energy between nanoparticles and surfaces. Using molecular mechanics and molecular dynamics simulations, we calculated the interaction of nanoscale rigid protein particles with nanostructured silicon surfaces of various sizes consisting of arrays of cones to mimic sharp, rough surface features inspired by the lotus leaf. Liquid water nanodroplets interacting with a similar set of surfaces were used to investigate the interaction for deformable particles. Binding energy, solvent-accessible surface area in contact between particle and surface, and wetting and repellency behavior were investigated. For rigid protein particles, simulations showed that the greatest binding energy was obtained between a particle and a flat, smooth surface. As the nanostructured cones increased in size, this interaction was reduced. The cone tips physically limited the interaction between particle and surface. For cone spacings and/or sizes greater than the size of the particle, it is expected the interaction energy will increase since the particle will "feel" flat surfaces. In the case of liquid water droplets in contact with similar cone systems, the wetting behavior was observed to slow down as cone density increased. It is expected that greater cone densities and more fractal length-scales (cones on cones) will lead to complete dewetting behavior of droplets larger than the cones. This work may help guide the design of future coatings for detection, protection, and decontamination applications.

Lotus Leaf

The lotus leaf is very clean because it is superhydrophobic. It's superhydrophobicity results from a very low binding energy to particles. The low binding energy results from the leaf being covered in forest of ~100nm pillars on ~10µm knobs, 30µm spacing. Can we design similar synthetic surfaces?



Applications



Spray-On Coating

www.neverwet.com

Self-Cleaning Clothes
(Dr. Quoc Truong, Natick)

www.army.mil/article/95276

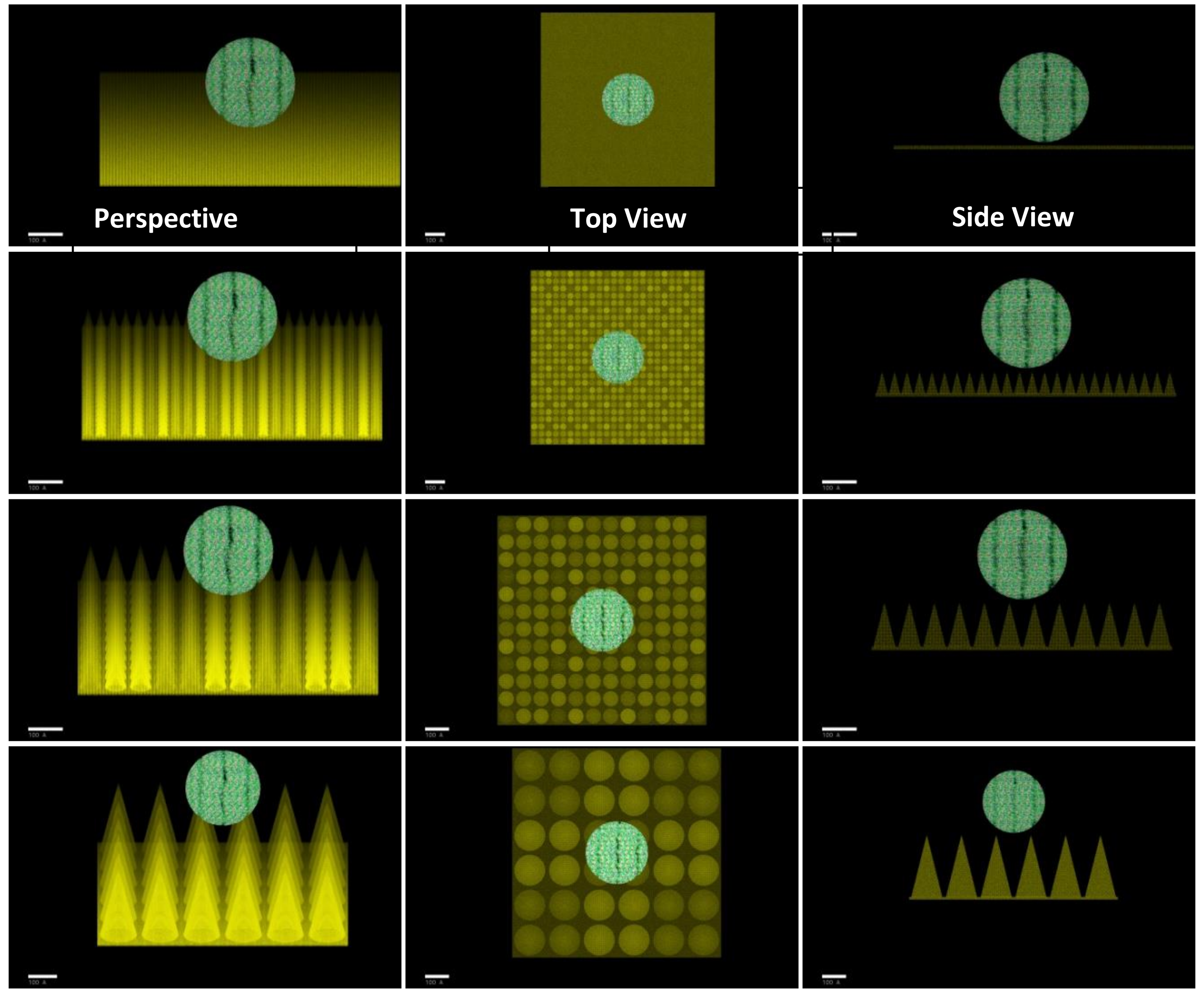
Detect

Protect

Decontaminate

Wikipedia and www.ecbc.army.mil

Rigid Protein Nanoparticle on Si



Models of a 26 nm protein particle interacting with nanostructured surfaces of varying cone size, beginning with a smooth surface (Top) and progressing to large, 26 nm high cones (bottom). Scale bar is 10 nm long.

Strongest binding energy observed when particle slips between cones

Key to a broadly repellant surface: *minimization of contact area*

Acknowledgements: The authors thank the Edgewood Chemical Biological Center for their assistance in this research and the U.S. Army for funding of this work through the In-House Laboratory Independent Research program. We also thank the Department of Defense Supercomputing Resource Centers (DSRCs) for High Performance Computing resources and the developers of LAMMPS and VMD. The views expressed in this presentation are those of the authors and do not necessarily reflect the official policy or position of the Department of Defense or the U.S. Government.

Water Nanodroplet on Si