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Theoretical and Numerical Modeling of faceted Ionic crystalline vesicles

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Icosahedral shape is found in several natural structures including large viruses, large fullerenes and cationic-anionic vesicles. Faceting into icosahedral shape can occur in large crystalline membranes via elasticity theory. Icosahedral symmetry is found in small systems of particles with short-range interactions on a sphere. Dr G. Vernizzi and I show a novel electrostatic-driven mechanism of ionic crystalline shells faceting into icosahedral shapes even for systems with a small number of particles. Icosahedral shape is possible in cationic and anionic molecules adsorbed onto spherical interfaces, such as emulsions or other immiscible liquid droplets because the large concentration of charges at the interface can lead to ionic crystals on the curved interface. Such self-organized ionic structures favors the formation of flat surfaces. We find that these ionic crystalline shells can have lower energy when faceted into icosahedra along particular directions. Indeed, the "ionic" buckling is driven by preferred bending directions of the planar ionic structure, along which is more likely for the icosahedral shape to develop an edge. Since only certain orientations are allowed, rotational symmetry is broken. One can hope to exploit this mechanism to generate functional materials where, for instance, proteins with specific charge groups can orient at specific directions along an icosahedral cationic-anionic vesicle.