Hexagulation numbers: magic numbers on the gyroid surfaces

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Regular structures of equal spheres on the gyroid minimal surfaces have been investigated as obtained through Monte Carlo simulations of hard spheres undergoing the Alder transition[1,2]. Remarkably, there exist magic numbers (Figure 1) producing regular structures, which are simply explained in terms of *hexagulation numbers* defined as $H = h^2 + k^2 - hk$, in analogy with the Caspar and Klug's *triangulation numbers* $T = h^2 + k^2 + hk$ for icosahedral viruses, where h and k are nonnegative integers[3]. The total number of spheres per cubic unit cell N is represented by $N = 16H$. Here we extend our simulations up to $H = 21$. When H is a multiple of three, we find that the space group $Ia\bar{3}d$ is broken into $I\bar{4}3d$, which is chiral with right- and left-handed version. These arrangements are analyzed in terms of the space groups, equivalent positions (Wyckoff positions), and polygonal-tiling representations (Figure 2). We also present bilayer regular structures composed of both right- and left-handed chiral layers having multiple of three H numbers.

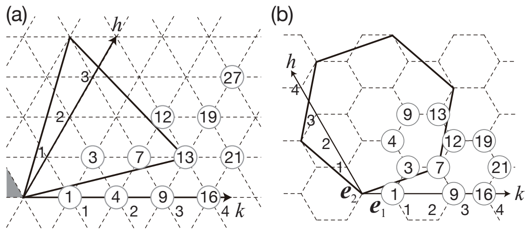

Figure 1 (a) Caspar and Klug's T-diagram for counting the triangulation number T and (b) H-diagram for counting the hexagulation number H. Lattice points denoted as (h, k) with h, k nonnegative integers in two oblique coordinate systems indicate circled numbers T=h^2+k^2+hk and H=h^2+k^2-hk: T is half the number of lattice points inside a triangle (solid line), while H is the number of dashed hexagons inside a hexagon (solid line). Shown here are T=13 with (3,1) and H=7 with (3,1).

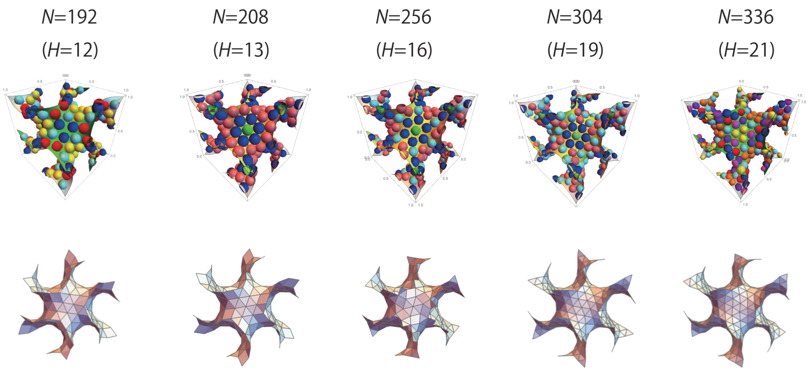

Figure 2 Top: Regular structures of hard spheres on the gyroid surface ($Ia\bar{3}d$). Bottom: their polygonal-tiling representations. H is the Hexagulation number and N is the number of spheres in a cubic unit cell. Colors indicate Wyckoff positions. Structures for H = 12 and H = 21 are chiral ($I\bar{4}3d$) having right- and left-handed version, both of which have been obtained by simulations.

The key is that only a limited number of efficient physical designs are possible even on negatively curved triply periodic minimal surfaces[4] like in icosahedral viruses. Future applications of such regular arrangements are to construct complex assemblies using the concepts of bijels, coloidosomes, polymersomes, and DNA-origami self-assemblies[5].

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