Soft Quasicrystals Optimize Sphere Packing

Stephan Förster[1], Martin Dulle[1], Vladislava Fokina[1], Thomas Gruhn[2]

[1] JCNS-1, Forschungszentrum Jülich, 52428 Jülich, Germany

[2] Biomaterialien, Universität Bayreuth, 95447 Bayreuth, Germany

Quasicrystals are a peculiar state of order, which is fundamentally different from classical ordered crystalline states. Discovered in 1982 for metal alloys, they have in recent years been reported for an increasing variety of non-metallic materials including polymers. However, no structural relations of the various non-metallic quasicrystals, as well as their connection to metallic quasicrystals have yet been identified. Such relations would provide important insights into the stability of quasicrystals. Here we show using simulations that spherical particles with soft repulsive interactions can form stable octagonal, decagonal, dodecagonal and icosahedral quasicrystals. We find structural agreement between simulated and experimentally observed two- and three-dimensional quasicrystalline structures and related tilings for polymers and nanoparticles investigated by us using X-ray and neutron diffraction, for all hitherto reported non-metallic quasicrystals, as well as for nearly all metallic quasicrystal types. We show that certain gyro-elongated bipyramids, which are close to the solutions to the Thomson problem, describe the three-dimensional arrangement of spheres in quasicrystals, suggesting that quasicrystals optimize sphere packing using two length scales. This furthermore explains the occurrence of exotic high pressure crystalline and quasicrystalline phases observed in meteorites and nuclear explosion sites. We demonstrate the practical applicability of this geometrical concept by fabricating colloidal quasicrystal on the photonic length scale exhibiting laser diffraction.