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Packings of Sphere Packings – an Unexplored Path to New Structures

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Sphere packings – three-dimensional arrangements of equal spheres with at least one uninterrupted path of contacts (bonds) between any two spheres – are prototypes of crystal structures. As such they are well-documented. Fischer, Koch and Sowa have enumerated homogeneous packings[1a] while a comprehensive database by O'Keeffe, Yaghi and coworkers covers heterogeneous ones as well.[1b] Surprisingly, composite sphere packings, or packings of sphere packings, have not been explored. Here two substructures must interpenetrate, contact being established between them without disrupting connectivity within either. This demands a degree of porosity and a symmetry relationship. While (self-) interpenetrating nets are not uncommon, contact between substructures – as observed in the trivial case of two interpenetrating diamond nets – does not occur as a rule. In fact, we now realize that the first nontrivial case of such a packing of sphere packings emerged only recently.[2] This new structure – a combination of the two univariant homogeneous sphere packings 4/3/c1 (**lcv**) and 3/10/c1 (**srs**) in $P4_132$ (213), with parameters $y(12d) = 0.1771$ and $x(8c) = 0.0363$ respectively (Figure 1c) – is, furthermore, found to possess a unique property. The density (0.648), the number of contacts per sphere (6) and the radial distribution function all closely mimick random close packing (RCP).[3] In other words it is the first structure which, although perfectly ordered, deserves to be called quasi-random.

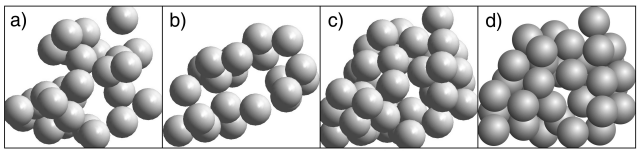

Figure 1. Portions of sphere packings: a) 4/3/c1 (**lcv**); b) 3/10/c1 (**srs**); c) composite of a) and b); d) random close packing after Bernal and Mason.[3a]

[1] a) H. Sowa, *Acta Cryst.* **2016**, *A72*, 357-365 and references therein; b) M. O'Keeffe, M. A. Peskov, S. J. Ramsden, O. M. Yaghi, *Acc. Chem. Res.* **2008**, *41*, 1782-1789.

[2] a) M. Petrik, W. Hornfeck, B. Harbrecht, *Z. Anorg. Allg. Chem.* **2014**, *640*, 2328; b) W. Hornfeck, P. Kuhn, *Acta Cryst.* **2014**, *A70*, 441-447.

[3] a) J. D. Bernal, J. Mason, *Nature* **1960**, *188*, 910-911, fig. 5; b) T. Aste, *J. Phys.: Condens. Matter* **2005**, *17*, S2361-S2390.

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