

Packings of Sphere Packings – a New Path to Solid State Ionic Conductors?

M. Petrik^{1*}, W. Hornfeck²

¹ Formerly Philipps-Universität Marburg, Vogelsbergstraße 13, 35043 Marburg, Germany;

² FZU, Institute of Physics of the Czech Academy of Sciences, Cukrovarnická 10/112, 162 00 Prague 6, Czech Republic

* The corresponding author; e-mail: spherepacker@gmail.com

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When hard spheres of equal size are packed together in space – meaning that any two spheres in the packing are connected by an uninterrupted path of close contacts – then this is a classical sphere packing. When, by analogy, entire sphere packings are imagined to be packed together – so that they interpenetrate each other and, without distortion, establish contact with each other – then this is what we call a *packing* of sphere packings (PSP) [1]. Note that the requirement of contact between the interpenetrating sphere packings rules out commonly known interpenetrating nets like MgCu_2 or Cu_2O .

Since the discovery of the first PSP (in the course of theoretical work on the β -manganese structure) [2] dozens of further PSPs have emerged and we have set up an online compilation, issuing at the same time a call for public contributions of new PSPs [3]. In view of the growing number of known PSPs the purpose of the present contribution is to call attention to the possibility that PSPs might provide new structural motifs conducive to free movement of ions in the solid state. A novel approach in the current quest for solid state ionic conductors applicable in rechargeable batteries is thus proposed.

We disregard the chemistry involved and consider only the structural aspects. Obviously a structure which permits free movement of ions must possess a sufficient degree of “openness” in the form of channels through which ions may pass unobstructedly. Now, the very nature of PSPs demands that already the primary sphere packings themselves possess a major degree of “openness” in order to leave enough room for interpenetration. But – and this is the point to be stressed here – even after interpenetration of the primary sphere packings it turns out that enough interconnected free space may still remain in the resulting PSP.

Two classic examples of superionic conductors illustrate this fact. (i) The structure of α -AgI (an intermediate-temperature silver ion conductor) is a PSP of iodine atoms – designated as PSP-1 [3] and consisting of two identical primary packings of the diamond type – in which a three-dimensional framework of channels remains open for the silver atoms to pass along freely. (ii) The structure of RbAg_4I_5 (a room-temperature silver ion conductor) is a PSP again of iodine atoms – now constituting a complex structure isopointal with β -manganese designated as PSP-5 [3] and built of two different primary packings – where again silver ions move freely in a three-dimensional framework of open channels.

References

- [1] M. Petrik, W. Hornfeck, *Z. Anorg. Allg. Chem.*, **642**, 1023 (2016)
- [2] M. Petrik, W. Hornfeck, B. Harbrecht, *Z. Anorg. Allg. Chem.*, **640**, 2328 (2014)
- [3] <https://spherepacker.github.io/welcome.html>, under “Sphere Packings.”