Deutsche Gesellschaft für Kristallographie DGK, 31st Annual Meeting, Frankfurt a. M., 2023.
(Adapted from the official book of abstracts, p. 128.)

Beyond Sphere Packings – *Packings* of Sphere Packings

Marek Petrik, formerly Philipps-Universitaet, Marburg, D;*
Dr. Wolfgang Hornfeck, Czech Academy of Sciences, Institute of Physics, Prague, CZ.

Rationalizing crystal structures in terms of sphere packings is an old tradition. While applying it to the structure of beta-manganese (β-Mn) we discovered a new way of using simple sphere packings to build more complex ones [1]. These we call *packings of sphere packings* (PSPs) [2]. The first PSP – isopointal with β-Mn, space group type $P4_132$, no. 213, Wyckoff positions 8c and 12d, x=0.03633 and y=0.17706 – was nearly identical with the iodine substructure of $RbAg_4I_5$, incidentally one of the best solid state ionic conductors known. After this initial discovery an exploratory search yielded dozens of other PSPs. An open online database was, therefore, set up and public contributions of PSPs were solicited [3]. This presentation will, it is hoped, arouse interest and promote further progress.

PSPs make two stringent demands on how the constituent sphere packings are combined: 1. each sphere packing must not lose any of its internal contacts, and 2. all sphere packings must establish contact among each other. The common types of interpenetrating structures, therefore, are ruled out since requirement 2. is not generally met, e. g. in Cu_2O or $MgCu_2$.

PSPs have so far been found of the cubic, hexagonal, tetragonal and orthorhombic type, the number of constituent sphere packings ranging from two to four. The goal is to discover different combinations of sphere packings yielding PSPs. *Different* combinations may, however, yield *the same* resulting structure. Thus not less than fourteen different PSPs all resulting in the fcc structure are listed by now [3].

Ultimately the challenge will be, given a complex structure like fcc or β-Mn, to enumerate all possible ways of splitting it into simpler sphere packings, subject to the two constraints stated above.

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

* Main author/presenting author
spherepacker@gmail.com