Poster Presentation

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Unique atom hyper-kagome order in structures of inorganic substances

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A unique atomic hyper-kagome order was discovered in spinel-like $Na_4Ir_3O_8$ crystal [1]. The Ir and Na atoms in $Na_4Ir_3O_8$ form two 3D networks of corner-shared triangles. Using group-theoretical, thermodynamic and structural methods of the Landau theory of phase transitions, we have proposed the general theory of the hyper-kagome atomic order in structures of inorganic substances [2, 3]. The formation of atom hyper-kagome sublattice in $Na_4Ir_3O_8$ is described theoretically on the basis of archetype (hypothetical parent structure/phase) concept. The archetype structure of $Na_4Ir_3O_8$ has a spinel-like structure (space group Fd-3m) and composition $[Na_{1/2}Ir_{3/2}]_{16(d)}[Na_{3/2}]_{16(c)}O_{32(e)}4$. The critical order parameter which induces hypothetical phase transition has been stated. It is shown that the derived structure of the $Na_4Ir_3O_8$ is formed as a result of the displacements of sodium, iridium and oxygen atoms, and ordering of sodium, iridium and oxygen atoms, ordering dxy, dxz, dyz – orbitals as well. Ordering of all atoms takes place according to the type 1:3. The Ir atoms form nanoclusters which are named decagons.

The existence of hyper-kagome lattices in six types in ordered spinel, pyrochlores and Laves phases (C15) structures is predicted theoretically. The structure mechanisms of forming predicted hyper-kagome atom order in some ordered spinel phases are established. For a number of cases typical diagrams of possible crystal phase states are built in the framework of the Landau theory of phase transitions. The proposed theory is in accordance with experimental data. It opens up new possibilities in the search for substances with anomalous physical properties, including superconductivity.

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