

Crystallographic patterns in three-dimensional euclidean space (E3) can be generated via orbits of motifs under the action of certain two-dimensional discrete groups acting in hyperbolic space (H2) followed by “wrapping” of the hyperbolic planar pattern onto three-periodic hyperbolic surfaces (e.g. minimal surfaces). This approach underlies the EPINET project [1] described in detail elsewhere [3], [4], [5].

We describe an explicit mapping between H2 and E3, mediated by three-periodic hyperbolic surfaces embedded in E3, that allows unique identification of a discrete hyperbolic group plus a surface with a space group.

The approach leads to the following concepts. First, point and plane groups describe isometries of the 2D sphere and euclidean plane respectively. Orbifolds offer a single coherent concept for point, plane and “saddle” groups, where the latter are isometries of H2. Second, we present a simple taxonomy of these groups into 8 classes via orbifolds, based on the generic topological and conformal structure of the orbifold. Third, we define crystallographic saddle groups (“sponge groups”) -- analogous to crystallographic point groups. These include those hyperbolic orbifolds whose orbits on embedded surfaces induce space groups in E3. We present a number of sponge groups within all eight classes, including the most symmetric example. These results allow many of the 230 space groups to be described in a concise manner, combining 2D isometries with surface topology.

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Crystal planes in Clifford geometric algebra

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Clifford’s geometric algebra [1] efficiently encodes geometric information in terms of compact algebraic expressions. These expressions allow to easily retrieve all geometric properties (radius, position, center, normal directions, orientation, distances, angles, ...), and one can simultaneously use these expressions as operators for transformations like reflections, rotations, roto-reflections, inversions (at points and spheres), roto-reflections, glide and screw transformations, etc. Products allow to combine objects, to intersect them, to compute their relative location and angles, etc. Thus geometric algebra has already been successfully applied to the description of crystallographic symmetry [2], [3]. We now extend this treatment by studying the description of offset subspaces in the geometric algebra of projective space $Cl(R^{n+1})$ and in the conformal model of Euclidean geometry, i.e. in $Cl(R^{n+1,1})$, see e.g. [4]. In particular, crystal planes in any dimension are such offset subspaces. The problem of defining a kD plane in terms of $k+1$ points on the plane is easily solved by taking the *outer* product of these points. Reciprocal vectors appear as support vectors of crystal planes, identical to the Euclidean parts of dual vectors describing hyperplanes in the above model algebras [5].

We mainly address crystallographers, who want to know how to successfully express their problems in the new comprehensive mathematical language of Clifford geometric algebra. We see a need for this, because so far many mainstream crystallographers are relatively unfamiliar with Clifford geometric algebra [6]. We focus on expressing key notions in standard crystallography, which clearly demonstrate how to employ the powerful invariant and dimension-

independent tools of Clifford geometric algebra. Thus we explain e.g. how to turn crystallographic *Miller indexes* into multivector expressions for crystallographic planes, and based on this how to directly compute crystal plane d -spacing, phase angles of structure factors, reflection conditions for the occurrence of Bragg reflections, interfacial angles, and the like.

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Symmetry relations and phase stability of magnesium borohydride $Mg(BH_4)_2$

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We studied the phase stability of $Mg(BH_4)_2$ by means of symmetry analysis of different structures optimized via first-principles methods [1]. In particular, we focused on the symmetry relations between space groups I41/amd (IT 141), I-4m2(IT 119) and F222 (IT 22) as one chain of subgroups and groups I41/amd (IT 141), Fddd (IT 70) and F222 (IT 22) as the second chain of subgroups. By that analysis, based on the theory of space groups and their representations (symmetry analysis method –SAM [2]) we found all transformations from the parent structure, described by the high symmetry group, to the structures with symmetries belonging to the appropriate subgroups. The main interesting result of the symmetry transformation provided the displacements of the atoms from their initial positions (by polar vector type SAM), and the ordering of clusters localized on given positions (by second rank tensor type SAM). The deformations of BH_4 clusters have been investigated by these two ways. Both vector and tensor type methods lead to the same description of ordering of deformed clusters, with the number of free parameters reduced to the same necessary minimum. Moreover this minimal number of free parameters has been used in the procedure of finding the lowest total energy for each proposed model of $Mg(BH_4)_2$ structure as follows. For every transformation from parent group to it subgroup, from symmetry point of view, each atom is allowed to move only in a strictly given direction (a displacement vector). This permits us to reduce the number of parameters we have to consider when looking for the minimum energy of the system under investigation. For example: the transition between groups (IT 141) and (IT 119) for $Mg(BH_4)_2$ in general is described by 264 free, independent parameters (88 atoms in the unit cell, each can move along x,y,z axis). Using the symmetry analysis this number is reduced to only 9 coefficients and in the case of transition between (IT 119) and (IT 22) this number becomes 12