Flat-branched semisimplicial complexes: a versatile tool for aperiodic solids

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We introduce flat-branched semisimplicial (FBS) complexes as a universal language to describe aperiodic structures of finite local complexity. An FBS-complex naturally represents the set of local atomic arrangements occurring in the structure. It includes both metric and combinatorial data; the flexibility of the latter allows for incorporation of structural constraints on a longer range. An FBS-complex can embody "local rules" of any kind, whether or not they impose a perfect long-range order. We propose an algorithm for exploration of local rules in terms of an FBS-complex directly from the phased diffraction data [1]. The FBS complex describing a structure entirely determines the density of atomic species, and yields experimentally verifiable constraints on their contribution to the structure factors [2].


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