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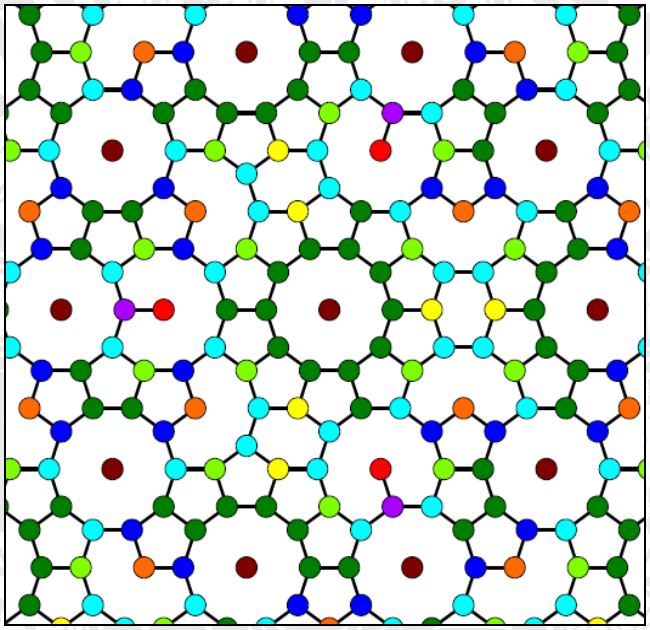

ENERGY OR ENTROPY: WHAT STABILIZES QUASICRYSTALS?

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Quasicrystals are ordered solids with point symmetries that are incompatible with translational periodicity. Their discovery in 1982 has been honored with the Nobel Prize for chemistry in 2011. The structure of quasicrystals can be described by aperiodic tessellations of space containing two or more types of tiles, as for example the Penrose tiling.
Quasicrystals carry a phason degree of freedom, which manifests itself microscopically by jumps between neighboring split positions. From the beginning of quasicrystal research it has been discussed, whether their stability is due to atomic interactions that favor matching rules for the tiles, or due to a high entropy caused by the phason degree of freedom [1]. We have established an atomistic model pair potential [2] which in molecular dynamics simulations gives rise to a two-dimensional, monatomic, decagonal quasicrystal (see figure). It has been possible to measure numerically the free energy of this system and to decide, whether their stability originates from energy or entropy [3].

[1] Elser V. 1989 in: Extended Icosahedral Structures, Eds. Jaric M.V. and Gratias D., pp. 105-136, Academic Press
[2] Engel M., Trebin H.-R. 2007 Phys. Rev. Lett. 98, 225505
[3] Kiselev A., Engel M., Trebin H.-R. 2012 arXiv:1210.4227v1