# Spontaneous formation of icosahedral quasicrystal from the melt in fully realistic atomistic simulation

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LOCATION: TU Vienna, Seminar Room 138C (Freihaus, Tower B/yellow, 9. OG)

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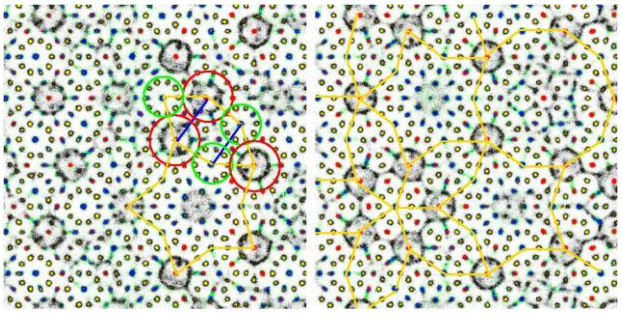
Recently, M. Engel et al [1] demonstrated self-assembly of icosahedral quasicrystals in a model one-component system, governed by parametrized oscillating pair potential (EOPP) [2].
I will show how the same type of interaction -- EOPP -- fitted to ab-initio forces in ternary Al--Cu--Fe alloy, spontaneously forms icosahedral quasicrystals in fully realistic replica-exchange atomistic simulation.

The quasicrystal phase is at high temperatures thermodynamically stable in a unique solid state, in which two kinds of small fundamental clusters permanently reshuffle, while maintaining icosahedral order in a flexible icosahedral network. The figure shows two snapshots of the high-temperature (1200K) structure separated by 2 ns time; the colors scale with occupancy probability by atoms (average over 0.5ns time). Red: Fe, yellow/gray: Al, green/blue : Cu.



[1] M. Engel, P. F. Damasceno, C. L. Phillips and C. Glotzer: {\it Computational self-assembly of a one-component icosahedral quasicrystal}; Nat. Mat. 2014, DOI 10.1038/NMAT4152\\
[2] M. Mihalkovi\v c, C. L. Henley: {\it Empirical oscillating potentials from ab--inito fits...}; Phys. Rev. B{\bf 85}, 092102 (2014)