



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

A talk by Marek Mihalkovic  
Institute of Physics, Slovak Academy of Sciences,  
Bratislava, Slovakia

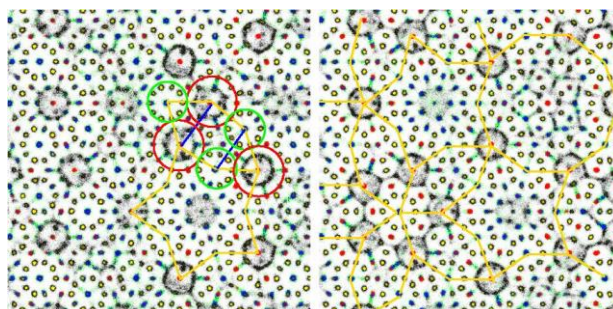
DATE / TIME: Monday, 26th of November 2018, 04:00 p.m.

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

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: *Computational self-assembly of a one-component icosahedral quasicrystal*; Nat. Mat. 2014, DOI 10.1038/NMAT4152

[2] M. Mihalkovic, C. L. Henley: *Empirical oscillating potentials from ab-initio fits...*; Phys. Rev. B **85**, 092102 (2014)