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Periodic crystals as local minimizers of atomistic energy functionals

How do periodic crystals emerge from (accurate quantum-mechanical or approximate) interatomic potential energy surfaces?

I will discuss open problems and recent progress, in particular identification of the 3D fcc (face-centered cubic) lattice as a local minimizer of the celebrated Lennard-Jones pair interaction model (joint work with Florian Theil, Warwick).

The analysis reveals a strong connection to stiffness of certain 3D nonlinear elastic networks.

More precisely one

– relates the atomistic energy to a (frame-indifferent, hence geometrically nonlinear) mass-spring network

– relates the mass-spring network to a (frame-indifferent) continuum energy; this involves a stiffness analysis for various few-atom 'tiles' such as equilateral simplices and equilateral octahedra

– applies a recent rigidity theorem (joint with S.Mueller and R.D.James) that the L2 distance of the gradient of a Sobolev map from the nearest rigid rotation is controlled by a constant times the L2 distance from the set of all rotations.