Der Wissenschaftsfonds.

Institut f. Analysis und Computational Number Theory (Math. A)

SFB-Kolloquium

Freitag, 19. 6. 2015, 14:00 c.t.

Seminarraum C 208, 2. Stock, Steyrergasse 30, TU Graz

Geometry optimization in carbon

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Carbon nanostructures such as graphene, nanotubes, and fullerenes are locally planar: each atom forms three covalents bonds which (ideally) create bonding-angles of $2\pi/3$. In distinguished regimes, this phenomenology can be modeled by minimizing specific atomic-interaction potentials including three-body interaction terms [T].

I intend to review some of the existing crystllization results for this kind of potentials [E,M,M2]. In particular, I will focus on the possibility of characterizing the geometry of energy minimizers, especially in three-dimensions. The stability, fine geometry, and partly the nanomechanics of classes of nanotubes and fullerenes will be discussed. This is joint work with M. Friedrich, E. Mainini, H. Murakawa, and P. Piovano.

[E] W. E, D. Li. On the crystallization of 2D hexagonal lattices. Comm. Math. Phys. 286 (2009) 1099-1140.

[M] E. Mainini, U. Stefanelli. Crystallization in carbon nanostructures. Comm. Math. Phys. 328 (2014) 545-571.

[M2] E. Mainini, P.Piovano, U. Stefanelli. Finite crystallization in the square lattice. Nonlinearity, 27 (2014) 717-737.

[T] J. Tersoff. New empirical approach for the structure and energy of covalent systems. Phys. Rev. B 37 (1988) 6991-7000.

E. Arrigoni, P. Grabner