Vienna School of Mathematics

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Variational Modeling of Molecular Geometries
(University of Vienna, Supervisor: U. Stefanelli)

Driven by their fascinating electronic and mechanical properties, research on low-dimensional materials (such as graphene) is exponentially growing. New findings are emerging at an always increasing pace, ranging from fundamental concepts to applications. In contrast to the wealth of experimental and numerical evidence currently available, rigorous mathematical results on local and global crystalline geometries are scant and the study of the emergence of different scales within molecular structures is still in its infancy.

The focus of the thesis project is on the variational modeling of molecular geometries: effective configurations are identified as minimizers of classical configurational potentials. This perspective allows to target a number of different issues including crystallization for molecular compounds, the description of local molecular features including defects and rigidity, the occurrence of global geometric characteristics such as flatness in three-dimensions and stratification, and the passage from discrete to continuum theories.

Tools will come from analysis, especially calculus of variations, and discrete geometry. The position is funded within an international cooperation project with Prof. Manuel Friedrich of the Applied Mathematics Group of the University of Muenster, Germany.

Applications have to be sent via the Job Center of the University of Vienna at the Reference number 10413. The deadline for application is **March 3, 2020**.