Einladung zum

Würzburger Mathematischen Kolloquium

Julius-Maximilians-Universität Würzburg • Fakultät für Mathematik und Informatik

Prof. Dr. Ulisse Stefanelli

University Wien

A variational invitation to carbon geometries

Mittwoch, 13. Apr. 2016 • 16:15 Uhr

Raum SE 40, Mathematik Ost, Emil-Fischer-Str. 40, Campus Hubland-Nord

Inhaltsangabe

Molecular Mechanics is an effective computational tool for simulating molecular structures and their chemical properties. Compared with quantum-informed models, it is seemingly the only practicable option when the size of the molecule scales up. This is particularly relevant for organic compounds, which can easily include hundreds of elements. Among these, I am specifically interested in pure-carbon molecules, the so-called carbon allotropes, presenting indeed a fascinating diversity of geometries and structures.

I intend to review some recent results on the variational modeling of pure-carbon ensambles. The focus will be on the rigorous descriptions of carbon geometries and their stability. In particular, I shall discuss the case of carbyne, graphene, some fullerenes, and diamond.

This is partly based on collaborations work with M. Friedrich, E. Mainini, H. Murakawa, and P. Piovano.

Zu diesem Vortrag laden wir Sie herzlich ein.
Im Anschluss an die Vorträge stehen Kaffee und Tee im Foyer vor dem SE 40 bereit.

Die Dozentinnen und Dozenten der Mathematik