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A variational invitation to carbon geometries

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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.