IMPRS UFAST

MAX-PLANCK-GESELLSCHAFT

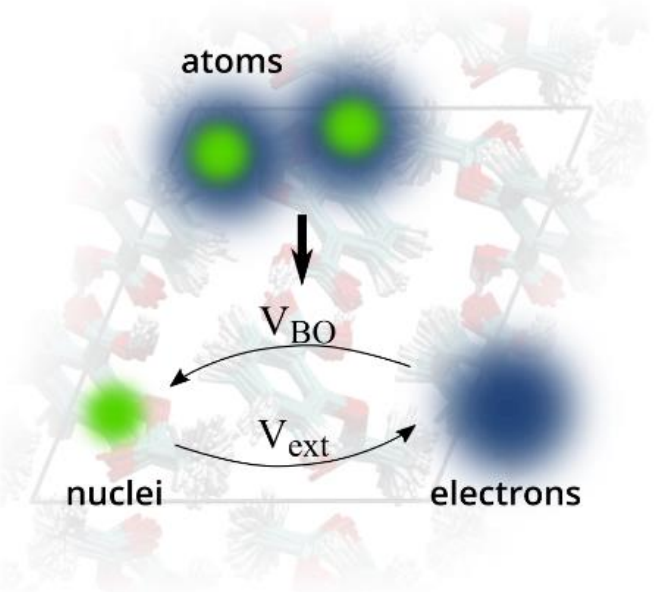
IMPRS UFAST Core Course

Theory of Electronic Structure and Molecular Dynamics (in the era of Machine Learning)

Mariana Rossi

Abstract:

The course will start by recapping the foundations and implications of the Born-Oppenheimer approximation and how it leads to the emergence of electronic structure theories. It will then cover the basics of wave-function based electronic structure methods, as well as electronic density based methods. Keeping with the Born-Oppenheimer approximation, we will then introduce concepts of statistical sampling and introduce different flavours of ab initio molecular dynamics as one of the methods to sample nuclear conformations within first-principles potential energy surfaces — and how novel machine learning techniques are transforming this field of computational research.



Meeting room O1.060

27th Feb. – 3rd March 2023

10:00 h – 12:00 h and

13:00 h – 16:00 h

Register on Geventis I-UF C5

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