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Ab Initio Approach to Ultrafast Spectroscopy with Stochastic Time-Dependent Density Functional Theory and Gauge-Including Projector Augmented Wave Method

Wednesday 3 July 2019 18:00 (2 hours)

We extend the gauge-including projector augmented wave method to the case of time-dependent electric fields of arbitrary strength and present its implementation in the VASP code. Interaction with an environment is described within the stochastic approach.

Authors: KRUCHININ, Stanislav (Universität Wien); Prof. KRESSE, Georg (Universität Wien)

Presenter: KRUCHININ, Stanislav (Universität Wien)

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