Computational Materials Science Seminar

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Online

# Three Christmas gifts for *ab initio* molecular dynamics

**Denis S. Tikhonov**

## Speaker introduction

Denis Tikhonov graduated from Lomonosov Moscow State University (LMSU) in 2014 (Specialist degree), Faculty of Chemistry, and later, in 2017, got his Ph.D. (candidate of chemical sciences degree) in Physical Chemistry from the same institution. For two years during his Ph.D., he worked at the University of Bielefeld (Germany), doing research in the fields of gas electron diffraction and molecular dynamics.

After Ph.D. Denis worked in an R&D lab at Geosplit LCC (Moscow, Skolkovo resident company) and also at the LMSU. In 2018, he went for a postdoc at DESY (Hamburg, Germany) to the group of Prof. Melanie Schnell, where he still resides. Denis's current scientific interests are femtochemistry, theoretical spectroscopy, quantum control of chirality, molecular dynamics, and experimental data analysis.

## Seminar abstract

*Ab initio* molecular dynamics (AIMD) is a nice tool to look into the nuclear motions of molecular systems.[1] AIMD and AIMD-based methods allow the calculation of structural and spectral properties,[2] finding chemical reaction pathways,[3] exploring molecular conformational landscapes,[4] and even tackling such hard tasks as mass-spectra prediction.[5,6] The main flaw of such simulations is the absence of the nuclear quantum effects (NQEs), which comes from the main assumption of the nuclei being classical particles.[2,7,8] Nevertheless, nowadays, NQEs are routinely introduced in AIMD simulations through different techniques, such as path-integral molecular dynamics (PIMD) and Wigner sampling [8].

## References

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Seminar

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