Centre for Research in Molecular Modeling
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Ab initio molecular dynamics on nanoscale

Despite remarkable recent progress in linear-scaling density function theory, the computational cost of existing methods remains too high for routine ab initio molecular dynamics (AIMD) simulations. We developed a new linear-scaling AIMD method with an extremely low computational overhead by assuming that electrons in materials are strictly localized within predefined radii. High efficiency of the method is achieved without sacrificing its accuracy with a combination of two techniques: (1) fast but only approximate description of localized electrons and (2) the stochastic treatment of nuclear motion, fine-tuned to retain stable dynamics even with imperfect forces. A remarkable feature of the implemented method is that it remains efficient for challenging condensed phase systems even if large accurate basis sets are used. We demonstrated that, for systems well-represented by localized electrons, the new AIMD method enables simulations on previously inaccessible time and length scales.

Rustam Z. Khaliullin obtained Ph.D. from the University of California at Berkeley. The focus of his research at McGill University is on the development of new theoretical methods and computational tools for solving difficult current problems in chemistry, solid-state physics, and materials science. His expertise extends from electronic structure methods and first-principle molecular dynamics to artificial intelligence methods and high performance massively-parallel computing for materials modeling. His group contributes to the development of multiple software packages including such popular codes as Q-Chem (quantum chemistry) and CP2K (materials science). He is particularly known for his first-principal studies of intermolecular interactions, especially those in liquid water.