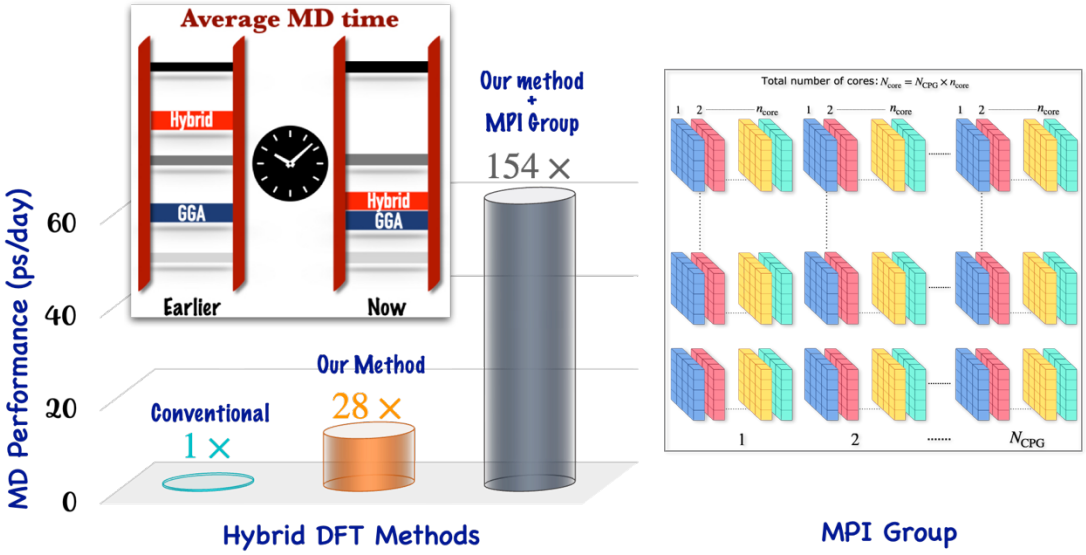
Molecular Dynamics Simulations at the Fourth Rung of DFT Functionals

Nisanth N. Nair

Department of Chemistry, Indian Institute of Technology Kanpur, Kanpur, 208016, India
**Email: nnair@iitk.ac.in*

Molecular dynamics (MD) simulations employing density functional theory (DFT) and plane waves are routinely carried out at the level of generalized gradient approximation (GGA). On the other hand, hybrid density functionals are more accurate and reliable than GGA functionals for predicting energetics and structural and dynamic properties. However, the computational cost for carrying out MD simulations using hybrid functionals and plane-wave basis sets is at least two orders of magnitude higher than that using GGA functionals for a system of ~100 atoms. Here we propose methods to reduce the computational cost of MD simulations with hybrid functionals to the extent that the computational cost is nearly the same as that with GGA. This development has made it possible to study the mechanism and free energetics of complex chemical reactions in condensed matter systems through very long MD simulations at the level of hybrid density functionals. I will discuss some of the recent



applications of the methods.

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