Center for Molecular Spectroscopy and Dynamics, IBS-Korea University

IBS Center for Molecular Spectroscopy and Dynamics

COLLOQUIUM

- **SPEAKER**
  Prof. Rustam Z. Khaliullin (Dept. of Chemistry, McGill University, Canada)

- **TITLE**
  Ab initio molecular dynamics on nanoscale

- **ABSTRACT**
  Despite remarkable recent progress in linear-scaling density function theory, the computational cost of exist-ing methods remains too high for routine ab initio molecular dynamics (AIMD) simulations. We developed a linear-scaling AIMD method with an extremely low computational overhead by assuming that electrons in materials are strictly localized within predened radii. High eciency of the method is achieved without sacricing its accuracy with a combination of two techniques: (1) on-the-y construction of accurate localized orbitals without lengthy optimization and (2) the stochastic integrator that is ne-tuned to retain stable dynamics even with imperfect forces. A remarkable feature of the implemented method is that it remains ecient for challenging condensed phase systems even if large accurate basis sets are used. We demonstrated that, for systems well-represented by localized electrons (e.g. molecular systems, ionic salts), the new AIMD method enables simulations on previously inaccessible time and length scales. Applications of the method to more challenging systems of strongly interacting atoms (e.g. covalent crystals) will also be discussed.

- **DATE AND VENUE**
  November 8, 2017 (Wednesday, 5:00 - 6:00 pm)
  Seminar Room 116, KU R&D Center

- **LANGUAGE**
  English

- **INVITED BY**
  Prof. Kyungwon Kwak

* If you want to have a discussion with Prof. Rustam Z. Khaliullin or have dinner with him, please contact Prof. Kyungwon Kwak (kkwak@korea.ac.kr).