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Special Issue on Molecular Dynamics Method

Call for Papers

Molecular dynamics (MD) is a computer simulation of physical movements of atoms and molecules in the context of N-body simulation and has become an important technique for the study of fluids and solids. In MD, the atoms and molecules are allowed to interact for a period of time, giving a view of the motion of the atoms. In the most common version, the trajectories of atoms and molecules are determined by numerically solving the Newton's equations of motion for a system of interacting particles, where forces between the particles and potential energy are defined by molecular mechanics force fields. Because molecular systems consist of a vast number of particles, it is impossible to find the properties of such complex systems analytically; MD simulation circumvents this problem by using numerical methods. With the MD method, not only the static quantities but also the dynamic quantities can be obtained.

In this special issue, we intend to invite front-line researchers and authors to submit original researches and review articles on exploring **Molecular Dynamics Method**. Potential topics include, but are not limited to:

- Molecular dynamics method
- Molecular dynamics simulation
- An initio molecular dynamics
- Equilibrium molecular dynamics
- Discontinuous molecular dynamics

Authors should read over the journal's Authors' Guidelines carefully before submission, Prospective authors should submit an electronic copy of their complete manuscript through the journal's Paper Submission System.

Please kindly notice that the "**Special Issue**" under your manuscript title is supposed to be specified and the research field "**Special Issue – *Molecular Dynamics Method***" should be chosen during your submission.

According to the following timetable:

Manuscript Due	December 26th, 2013
Publication Date	February 2014

Guest Editor:

For further questions or inquiries
Please contact Editorial Assistant at
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