

To Dr.Ling Miao  
Editor of Physical Review X

Luigi Delle Site  
Heisenberg Fellow  
Institute for Mathematics,  
Freie Universität Berlin  
Arnimallee 6, D-14195 Berlin  
Tel: (030) 838 75367  
Fax: (030) 838 75412  
e-mail:  
luigi.dellesite@fu-berlin.de

## Submission of a manuscript

Dear Dr. Miao

We would like to submit the paper entitled: *"The Reliability of the Adaptive Resolution Technique in Performing Grand Canonical-Like Molecular Dynamics Simulations"*, by H.Wang, C.Hartmann, C.Schütte and myself, to Physical Review X for publication. The main quality of the paper lies in its multidisciplinarity, that is the use of a rigorous mathematical formalism in translating physical principles and hypothesis into an efficient numerical protocol for molecular dynamics (MD) simulation of liquid systems. Also the practical results are, in our view, rather interesting: (1) we prove that the adaptive resolution approach is in fact (up to some order) a Grand Canonical framework for the (small) high resolution region. We also provide the mathematical criteria to rigorously define the order of accuracy and (eventually) show how to reach high orders in a systematic way; (2) our method, contrary to other Grand Canonical MD methods, does not require the a priori knowledge of the chemical potential. This latter for liquid systems is very difficult to obtain either for the high computational costs required and/or for the accuracy that one can reach in its calculation.

In our view this work is the results of an optimal combination of different disciplines, mathematics, physics, chemistry and computational science, with solid conceptual results, but also very practical consequences regarding the applications in MD. For this reason we believe that PRX may provide the broad visibility that multidisciplinary approaches need in order to be promoted across the different communities.

As potential referees we suggest the following scholars:

- Christoph Dellago, University of Vienna
- Edward Maginn, University of Notre Dame
- Marina Guenza, University of Oregon
- Donald Truhlar, University of Minnesota
- Cecilia Clementi, Rice University
- Cameron Abrams, Drexel University
- Mark Tuckerman, New York University

- Will Noid, Penn State
- Daan Frenkel, University of Cambridge
- Sara Bonella, University of Rome

Thank you for the attention.

Sincerely Yours

Luigi Delle Site  
(On behalf of all authors)