Dear Prof. Du:  
  
Manuscript ID CP-PER-11-2011-023700  
Title: Quantum Chemistry Simulation on Quantum Computers: Theories  
and Experiments  
  
  
Thank you for your submission to Physical Chemistry Chemical Physics, and I apologise sincerely for the very long delay in the handling of your manuscript. Both referees have additionally apologized for any inconvenience caused.  
  
We have now received the reviewers’ reports on your manuscript, which are copied below. The reviewers feel that while the topic is of high interest and a nice piece of work, however, they feel that major modifications are necessary before publication can be considered. Referee 2 has sent in an annotated PDF of your manuscript, which I attach to this e-mail. Referee 2 has also raised concerns that the paper focuses too much on the work of two groups. While this is a Perspective, and focus on the author groups is expected, you should try and put the work in the context of the research area as a whole in your revised manuscript.  
  
Based on the reviewers’ comments publication of your manuscript in its present form is not possible. However providing that the comments of the reviewers are addressed in full I will be pleased to consider a revised manuscript. The manuscript will be subject to further peer review prior to reaching a final decision on acceptance.  
  
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Once again, thank you for submitting your manuscript to Physical Chemistry Chemical Physics and I look forward to receiving your revision.  
  
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Advanced Articles from new RSC journal, Catalysis Science & Technology are now freely available online.  
  
Reviewers' Comments to Author:  
Referee: 1  
Comments to the Author  
This paper deals with quantum simulations toward quantum chemistry, both theoretically and experimentally on a small quantum computer. The authors have attempted to persuade us to anticipate that the quantum simulation itself will provide us with a powerful quantum chemistry tool over computations by classical computers, emphasizing that quantum simulations can have intrinsic advantages over classical computations. In most of the sections, the relevant issues have carefully been chosen and elaborately described for non-specialists, except for 2.2.2. Indeed, the references have been cited, but a more detailed description will be necessary for non-specialists. The addition will strengthen the MS and improve the quality. In Fig. 4(b), the units description is not correct according to the IUPAC/IUPAP conventions. Totally, the MS is a nice piece of work as “Perspective.”  
  
Referee: 2  
Comments to the Author  
Referee report for:   
  
CP-PER-11-2011-023700 - Quantum Chemistry Simulation on Quantum Computers: Theories and Experiments  
  
The topic of this review is an excellent choice, and the authors are top-level in this field. Thus, I am very positive about this manuscript.   
  
However, there are many problems with it. So many that I began typing these, but it took forever to describe these in writing as a long list (page x, first column, line Y from the top, …. etc. etc.).  Thus, I decided to write the changes directly into the manuscript, so it would be easier to identify what to change and where to introduce the change.    
  
Some referee reports do not provide specific suggestions to improve a manuscript. Just generalities. These reports are not very useful to authors. It is better to provide many specific and detailed examples of places where the paper could be improved. The attached PDF file has more than 200 very specific suggestions on how to improve the manuscript.  After these changes are implemented, the authors might wish to try to improve the manuscript a bit further. I guess that the editor might have to edit the text further, towards the end. However, this first pass might make further changes easier to implement.   
  
Some parts of the review seem to be a bit too long. For instance, the quantum optics implementation described in section 3.2 has been described by the people who did that work and by top experts on this as “the most expensive way to diagonalize a 2x2 matrix” and the text of the review should describe that work using those words inside the quotation marks, because these convey the reality of that paper, which has been oversold to the press.  Indeed, that paper was rejected by several journals, before it was published, because it was ill-designed. It takes a simple task (diagonalizing a 2x2), and transforms it into a massively messy one, with complex optics and also classical computers helping the process.  It is surprising that section 3.2 would devote so much space to “the most expensive way to diagonalize a 2x2 matrix”.   
  
Section 4.2 also devotes too much space to ref. 60, which is over-emphasized there. Namely, papers that have been oversold before, are still overrated here.   
  
The reference section could be more balanced. Now it is dominated by two groups: HU and USTC.  Same with the text of the review: too much emphasis on works by these two groups, specially HU. Yes, these two groups have done considerable work in this area, but too much focus on two groups makes the review less appealing to a broader audience. Also, the excellent USTC work has not been oversold to the press, in my opinion, but the one from HU has been, according to many. Different (boasting) styles.   
  
In summary, the topic of this review is an excellent choice, and the authors are top-level in this field. This review has many positive aspects and I recommend it to be published AFTER significant changes are introduced. It is not just English grammar, but much more than this. More care is needed. More attention to detail is necessary. For instance, the figures in the paper do not have references, and these are often indicated (in the best reviews) as “This figure is reproduced from ref. X”, so the reader of each caption would immediately know where the figures are taken from.     
  
In addition, some sentences are clearly incomplete. Other sentences are too long and better be split. Other sentences are confusing. I tried to fix many of these problems, and other issues, over 200 times, but I am sure that many additional changes are needed. My suggested changes will significantly improve this paper, but more improvements are needed. I cannot write these all here, because otherwise I would be rewriting the entire manuscript, which I do not wish to do (although I am getting closer to it).