



Message from the TSTC Founder, Jack Simons

Hi, this is Jack Simons speaking, and I am addressing you because you have either signed up to attend a Telluride School on Theoretical Chemistry (TSTC; <http://www.telluridescience.org/tstc>) or you may be interested in doing so. I want to explain what these schools are all about and why I founded them in 2008.

Most of you have focused your efforts on problems of current importance within one of the following fields: electronic structure theory, biological molecule or materials simulations, chemical reaction dynamics, or statistical mechanics. You have probably taken introductory graduate level courses covering most of these topics, but your research-level expertise is likely limited to the specific field within which you are currently working.

Largely due to the advent of high speed computing, our field of theoretical chemistry underwent explosive growth between the 1960s and the present, and is having more and more impact within the chemistry, materials science, biology, atmospheric science, and physics communities. I believe this trend will continue during your scientific career, as a result of which you will be presented with an amazing range of opportunities to employ the tools of theory to solve important and exciting problems in many areas of science. However, to do so, I think you will be best served if you build a broader and deeper background than you probably now possess within the areas of theory where you have not yet carried out research-level work. It is primarily to help you begin to build such a firm background that we offer TSTC.

We want those of you working in electronic structure theory to learn, at a level beyond graduate classes, about molecular simulations, reaction dynamics and statistical mechanics so you know, for example, about biomolecule force fields, solvation models, surface hopping methods, tools for sampling rare events, etc. Likewise, we want those of you working on biomolecule simulations to learn about density functional, Hartree-Fock, and coupled-cluster theory, and about conical intersections and surface hopping. That is, we want to provide each of you with an efficient route for learning enough about the other fields of theoretical chemistry that, as opportunities arise in your future career adventures, you will feel confident about delving even more deeply into these areas so you can apply their tools to scientific challenges you want to pursue.

So, the main purpose of TSTC schools is to offer you exposure to Ph.D. level background material in the areas of theory within which you are currently not working. If you want learn more about your specialized area of emphasis within theory, I suggest that you consider attending one of the many Telluride Science Research Center workshops (TSRC; <http://www.telluridescience.org/>) offered each year.

I understand that one intense week of exposure to such subject matter will not bring you to a cutting-edge research level (we intend to expand the TSTC schools to two weeks once we have adequate funding) of knowledge. However, I believe that, if you work hard to assimilate the material offered in TSTC, you can achieve a broadening and deepening of your background that will serve you well in your future research endeavors. I want you to know that I and the other theoretical chemists who have volunteered to teach in TSTC schools care deeply about our discipline and about you as its future leaders. If you attend TSTC, we hope you enjoy your experience, learn a lot, and create networks with other members of theoretical chemistry's future. We are doing our best to offer you a unique opportunity, and we ask that you do your best to master the material presented at TSTC.

I wish you the very best in your exciting young career.

Sincerely,

Jack Simons