Announcement of a Workshop at the Aspen Center For Physics

“Molecular Physics of Non-Bonded Biomolecular Interactions”

Summer 2013

A proposal is being submitted to the Aspen Center for Physics (ACP) in Aspen Colorado to sponsor a three week workshop focusing on efficient computational approaches to enhance the understanding of non-bonded interactions in biological systems and assemblies.

Non-bonded interactions are integral to biological processes ranging from ligand-active site binding, through protein and polynucleotide folding and assembly, and to cell membrane permeability. Despite their ubiquitous nature, efficient and accurate computational methods to model such interactions remain a challenge. In addition, the fundamental quantum mechanical nature of certain classes of non-bonded interaction, such as hydrogen bonds and more recently the analogous halogen bonds, remain debated topics. This Aspen Center for Physics workshop will focus on efficient computational approaches that help to enhance our understanding of non-bonded interactions in biological systems and assemblies. Efforts will be directed at improvements in long-range electrostatic interactions, medium range dispersive and charge transfer interactions, as well as short-range hydrogen bonding and the exchange repulsion term.

The workshop will occur sometime during the last two weeks of June through the end of July of 2013 depending on space availability.

The purpose of this advertising statement is to find 40 Ph.D. scientists that may have interest in such a workshop. However, no commitment is required at this time. If the workshop is accepted, ACP will notify interested parties and put out a general invitation and application on their web site.

The purpose of the ACP is to provide an enriching and non-interrupted atmosphere for each person to work on an individual project while having time to exchange ideas with other attendees. The workshop is partially funded by the National Science Foundation through significant reductions in housing costs. There are no experimental facilities at ACP so all projects are computational in nature. More information on the goals and costs of attending the workshop can be found on the ACP web site – aspenphsy.org.

Formal presentations on individual work are not required. However, short presentations are encouraged at the beginning of the workshop for introductions as to the expertise of each attendee.

The workshop is being organized by the following people who have interests, respectively, in modeling of protein folding, macromolecular structure through halogen bonds and force field development:

Dr Mark Plummer – **MP***r&d*, LLC - [mplummer65@msn.com](mailto:mplummer65@msn.com)

Dr. P. Shing Ho – Dept. Biochemistry & Mol. Bio., Colorado State University – [shing.ho@colostate.edu](mailto:shing.ho@colostate.edu)

Dr. Anthony Rappé – Dept. Chemistry, Colorado State University – [rappe@lamar.coloradostate.edu](mailto:rappe@lamar.coloradostate.edu)

Please contact one of the above by June 29, 2012 to express an interest and a possible area of study.