Special Issue

Novel Algorithms/High Performance Computing Arising in Molecular Electronic Structure Theory

Message from the Guest Editors

This Special Issue will consist of manuscripts describing recent advances in the understanding and prediction of the electronic structures of molecules. Many of these advances are concurrent with the development of new algorithms and deployment of existing algorithms on new architecture. Manuscripts that describe new methods for strong correlation in molecules (or molecular fragments) that avoid the steep factorial scaling of fully variational methods are particularly encouraged (e.g., stochastic models). The Special Issue is expected to include submissions on molecular properties, including relativistic effects and the practicable inclusion of quantum electrodynamics (QED). Many of the new developments make extensive use of GPUs and other architectural advances in computers.

Guest Editors

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Deadline for manuscript submissions

closed (30 June 2019)

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You are invited to submit the results of your research for consideration and publication in *Computation,* an international open access journal, which is published monthly online by MDPI.
The editorial board and staff of *Computation* are dedicated to establishing a benchmark journal for the world scientific and engineering communities for original research articles, reviews, conference proceedings (i.e., peer reviewed full articles), and communications, in the cutting-edge areas of computational biology, computational chemistry, computational social science and computational engineering.

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