Enabling High-Throughput Material Screening Based on Dynamic and Transport Properties

DMREF/HydroGEN EMN Postdoctoral Position

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The Materials Genome Initiative and related efforts have demonstrated the value of large-scale computational screening of candidate materials for a wide range of applications. Particularly relevant to the proposed work is the Electrolyte Genome Project (JCESR) where candidate electrolyte molecules are winnowed by redox potentials, solvation energies, and structural changes. All these properties can be estimated with accuracy using *ab initio* methods; however, transport properties crucial to the performance of batteries and related electrochemical devices cannot. Here, molecular dynamics is the appropriate tool and can estimate diffusion coefficients, viscosities, mobilities, and other dynamic properties as well as performing large-scale, dynamic solvation analysis.

We propose a project complementary to the Electrolyte Genome in line with the goals of the Designing Materials to Revolutionize and Engineer our Future (DMREF) and Materials Genome Initiative (MGI) programs to (a) create computational machinery necessary for large-scale material selection based on Sandia's LAMMPS exascale molecular simulator and (b) target the development of optimal ionomer/ionic liquid based electrolytes for batteries and hydrogen production. The work will include developing:

- Software to transform molecular structures to viable molecular models with interaction forces, partial charges, etc. without supervision.
- Efficient/accelerated means of equilibrating solute-solvent mixtures that may be near glass-transition temperatures and methods to assess equilibration and statistical independence of replica systems.
- Means of validating molecular models of electrolytes prior to property prediction and means of adjusting potentials to improve accuracy.
- Sampling, convergence, and machine learning techniques to manage the high-throughput data coming from Green-Kubo and related techniques.

All these developments will be tested and applied to both simple systems, for validation, and ionomer/ionic liquid based electrolytes, for technologically relevant predictions and hand-off to experimental investigation.