Collaborative Research: Frameworks: Enabling reproducible research in soft materials with the Multiscale Polymer Toolkit (MuPT)

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Need: Progress in polymeric soft materials research is hindered by the lack of computational tools that can simultaneously represent the molecular relaxations and chemical reactions that influence morphology in biogels, aerospace composites, separation membranes, and vitrimers. Meeting this need requires interdisciplinary scientific software development leveraging expertise in force field parameterization, coarse-graining, polymer physics, reaction dynamics, and data structure development for high performance computing across multiple simulation engines and hardware architectures.

Vision: The Multiscale Polymer Toolkit (MuPT) will enable reproducible, extensible computational research on reacting polymer materials that spans Ångström-to-micron length scales through open software libraries and community recipes.

Developer Community: Built through involvement in previously funded ecosystems of tools *MoSDeF* (Jankowski, CSSI), *PolymerizeIt!* (Sarupria, DMREF), *Polymatic* (Sampath, DMR), *REACTER* (Gissinger, NASA), *OpenFF* (Shirts, NIH), and simulation engines *HOOMD-Blue* (Jankowski), *GROMACS* (Shirts), and *LAMMPS* (Gissinger). **Application Community:** Polymer researchers across academia, national labs (including NREL, LLNL, INL, NIST), industry (including Boeing, and Toray) and international consortia (CECAM, FairMAT). Particular focus on reacting and reconfigurable polymer materials areas including plastic recycling, structural composites, separations, biogels, and scientific computing communities where high-throughput studies and machine learning of higher-order models have urgent need. **Approach:** Open Molecular Software Federation software developers pair with domain experts (graduate students, PI's) to develop software and tutorials. Findability and accessibility will be accomplished through conda-forge deployment and public workshops.

Deliverables:
(a) A multiscale internal software representation for polymers, enabling exact data conversion between simulation engines representations at the same resolution scale, and tools for lossy conversion to coarse-grained representations, and inferring representative higher resolution representations.
(b) An API for this representation, allowing researchers to interface existing software tools for polymer parameterization, building, and crosslinking, with robust error catching.
(c) A workflow API that allows chaining of existing software tools, enabling users to programmatically generate simulation engine inputs by specifying simulation engine, chemistries, reaction models, and molecular representations.
(d) A searchable repository of community-vetted polymer simulation workflows, initially seeded and maintained by the PI's of the grant.
(e) Documentation for best practice in polymer modeling, with examples using the workflow.
(f) Improved materials and recommendations for training research software engineers.

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Urgent Challenges and Applications: (1) programmatic generation of polymer morphologies and their forcefield parameterizations, including support for thermosets, polymer conjugates, composite materials, copolymers and blends; (2) automated analysis tools for common polymer properties, such as strength/modulus, T_g, dispersity, alignment/crystallinity, structure factor and porosity; (3) generation and screening of novel polymer chemistries for a particular objective function, such as strength of a composite or selectivity of a membrane; (4) curating data with interchangeable atomistic and coarse-grained representations for multilevel discovery and design, and (6) optimizing processing conditions, e.g., temperature and pressure, for difficult-to-manufacture functional materials, such as aerospace composites.

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