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An Integrated Computational and Data Environment to Support Multiscale Modeling of Soft Materials for the Materials Genome Initiative FREDERICK PHELAN JR., THOMAS ROSCH, CHEOL JEONG, BRIAN MOROZ, SHARIEF YOUSSEF, NIST - Natl Inst of Stds Tech — In this presentation, we describe the development of a computational "workbench" whose goal is to provide an integrated computational and data environment to support multiscale modeling of soft materials for the Materials Genome Initiative (MGI). The design has three essential elements: a modular program structure that supports the addition of new functionality through Python scripting and run-time plugins; a hierarchical data structure which enables unified representation of materials at different levels of granularity; finally, integration of the NIST Materials Data Curation System (MDCS) into the environment to support ontology based materials descriptions. The feature of the workbench which we emphasize in this presentation is coarse-graining. Coarse-graining techniques are an essential requirement for the design of soft materials, and are an active area of research across the soft matter community. We illustrate how the approach allows the integration of multiple coarse-graining techniques in a common environment to greater enable development, evaluation and comparison of new algorithms. Moreover, the environment meets the goals of the MGI by enabling automated curation of both upstream and downstream data in materials reference libraries which can be pushed or shared by various means.

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