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Cyber Infrastructure for Exploring Novel Polymeric Materials

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We are in the process of building a global cyberinfrastructure (CI) for exploring and predicting structural and dynamical properties of complex materials. Such a CI for materials has the potential of integrating, for the first time, the diverse knowledge of the world's experts in materials science and engineering. Through such collaboration, seemingly disparate theories and experimental observations will be linked and taken to their limits, thereby leading to unexpected insights and new questions. At the current state, the CI focuses on applied and theoretical rheology. We envision a global alliance of rheology experts who access each other's experimental results, make predictions with each other's theories and simulate with each other's computer codes. At the center of the CI is a platform operating system (IRIS code, see <http://rheology.tripod.com/>) that connects a wide range of dedicated software modules. These CI modules perform calculations and return the corresponding results to a central graphics screen. A universal data standard unifies data from heterogeneous sources and facilitates communication between laboratories worldwide. Several of the world's leading rheology experts have begun to write theory modules that seamlessly connect into the rheology CI; several modules are complete and more are in progress. The rheology CI helps with tasks such as materials development, polymer engineering applications, teaching of rheology, rheology research (experimental and theoretical), data communication and archiving. The tools will allow industrial users to adjust rapidly to the changing needs and the pressure to obtain short-term solutions in a competitive environment. Untrained talent gets introduced quickly into the most advanced concepts of material structure and dynamics.