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Chemistry Unified Language Interface: a Novel Toolkit for Hybrid Macromolecular Models

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In our everyday life, we appreciate the enormous diversity of industrial formulation in many applications, from personal and health care, to plastics and coatings, to novel nanotechnology. In all of these cases the systems are compound, containing solvents mixtures, polymers, surfactants, actives and colloids or fillers. CULGI (Chemistry Unified Language Interface) is a library of many modeling functions and approaches, encompassing molecular, mesoscopic and macroscopic chemical modeling and machine learning. We discuss several of the important theoretical challenges that we face: (a) the lack of unification in classification and description of common chemical entities, such as molecules, colloids and surfactants, (b) the curse of loss of thermodynamic accuracy in large scale molecular dynamics, and (c), most importantly: how to derive interaction models and parameters for real mixed systems of industrial relevance on a coarse-grained level. We illustrate the challenges by some resent results relevant to industrial formulation and application: the in situ phase formation of polyolefin blends, the lyotropic phase structure of concentrated surfactant ? polyacid mixtures, and dissolution rates of sparingly soluble drugs from polymer stabilized suspensions.