Towards a universal model of the liquid phase: How to have it all

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The geological and planetary communities need those of us that work on silicate liquids to provide a simple, reliable product: an accurate predictive model of the chemical, dynamical, and transport properties of multicomponent liquids of arbitrary composition at any (often extreme) pressure and temperature. Such a model would be used (with similar models of solids and vapors, and perhaps coupled to dynamical models of all kinds) to construct scenarios or invert for conditions describing all the magmatic phenomena that affect planetary evolution, volcanic hazard, ore genesis, etc. This is a noble goal and a grand challenge. How close are we, and how can we chart a path to get there?

A variety of approaches have been pursued. Experimental observations are essential — empirical models cannot be built and *ab initio* models cannot be tested without them — and observational efforts using established and new methods must continue. But observation alone is insufficient; we need models that hindcast the observations but also forecast under conditions that cannot be or have not been observed, at the speed of numerical and thought experiments. Such models fall into two large classes: thermodynamics and molecular dynamics (MD). Each has its strengths and weaknesses.

MD models, whether fully classical (with empirical force fields) or semi-classical (quantum electrons coupled to Newtonian nuclei) remain too inefficient to provide output quantities in real time; even if exactly correct (which they are not), they need to be parameterized and so the same issues that arise in paramerization of experiments arise. Classical thermodynamic models inevitably reflect simplifying choices driven by either computational efficiency or by limits in quantity, precision, and internal consistency of calibration data, which from time to time must be re-examined as more and better computational power and data become available.

Inspired by recent MD results, spectroscopy, and shock compression results, we are building paradigms for continuously differentiable and fast models with internal thermodynamic optimization that link short-range order and variable cation coordination to macroscopic observables. These are early steps, but extension to full multicomponent systems should lead to models that support confident extrapolation.