Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Liquid-state integral equations via the self-consistent field approach ISSEI NAKAMURA, State Key Laboratory of Polymer Physics and Chemistry, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, ZHEN-GANG WANG, Division of Chemistry and Chemical Engineering, California Institute of Technology — We develop liquid-state integral equations via the self-consistent field approach. Taking electrolytes and van der waals fluids as examples, we provide a generic procedure to bridge the longstanding gap between the self-consistent field theory and other multi-scale theories such as the density functional theory and the integral equation theory, and thus a major improvement on the statistical field theory. Our new self-consistent filed theory simultaneously accounts for many important features in soft matters, the molecular interactions at an atomic scale that are expressed beyond a mean-field form, the equation of state, the liquid-vapor phase coexistence, and the oscillatory behavior of the pair distribution function in a liquid phase and the monotonic decay of the pair distribution function in a gas phase.

Issei Nakamura
State Key Laboratory of Polymer Physics and Chemistry,
Changchun Institute of Applied Chemistry, Chinese Academy of Sciences

Date submitted: 14 Nov 2013 Electronic form version 1.4