Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

A Variational Statistical-Field Theory for Polar Liquid Mixtures[1]

BILIN ZHUANG, ZHEN-GANG WANG, California Institute of Technology — Using a variational field-theoretic approach, we derive a molecularly-based theory for polar liquid mixtures. The resulting theory consists of simple algebraic expressions for the free energy of mixing and the dielectric constant as functions of mixture composition. Using only the dielectric constants and the molar volumes of the pure liquid constituents, the theory evaluates the mixture dielectric constants in good agreement with the experimental values for a wide range of liquid mixtures, without using adjustable parameters. In addition, the theory predicts that liquids with similar dielectric constants and molar volumes dissolve well in each other, while sufficient disparity in these parameters result in phase separation. The calculated miscibility map on the dielectric constant-molar volume axes agrees well with known experimental observations for a large number of liquid pairs. Thus the theory provides a quantification for the well-known empirical like-dissolves-like rule.

[1]BZ acknowledges the A-STAR fellowship for the financial support.

Bilin Zhuang
California Institute of Technology

Date submitted: 06 Nov 2015 Electronic form version 1.4