

# The local dielectric permittivity in multi-component systems: Theory and Applications

R. Ramprasad

*Department of Chemical, Materials & Biomolecular Engineering,  
Institute of Materials Science, University of Connecticut  
Storrs, CT, USA*

A computationally efficient method within the framework of density functional theory to aid in the study of the dielectric properties of multi-component systems, with explicit treatment of surface and interface effects,<sup>1</sup> will be presented. The local polarization and permittivity functions, induced due to a finite external electric field, are introduced to describe variations of the dielectric response over length scales of the order of interatomic distances. This method allows for a partitioning of the net field induced polarization in nanoscale systems into bulk and surface/interface parts. In addition, this new procedure allows for the treatment of both the high frequency effects (when only the electrons are allowed to respond to the external electric field, while the ionic cores are held fixed) and low frequency effects (when both the electronic and ionic degrees of freedom are allowed to relax). Application of this method to several 1-component,<sup>2,3</sup> 2-component,<sup>1,2,3</sup> and molecular composite<sup>4</sup> systems will be discussed.

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