First principles theory of the local dielectric permittivity: Application to surfaces and interfaces NING SHI, RAMPI RAMPRASAD, Department of Materials Science and Engineering, Institute of Materials Science, University of Connecticut, 97 N. Eagleville Road, Storrs, CT 06269 — A new computationally efficient method has been developed 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. The local polarization and permittivity functions, induced due to a finite external electric field, are introduced to describe variation of the dielectric response over length scales of the order of interatomic distances. Specially, we have determined the position dependent dielectric permittivity profiles for Si-SiO$_2$ and SiO$_2$ -polymer systems. We find that at regions close to surfaces and interfaces, the dielectric permittivity is enhanced compared to the corresponding bulk values, while in interior regions it approaches the corresponding bulk values. The calculated optical and static dielectric constant values of these systems are in excellent agreement with experimental results, and other more involved computational treatments.

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