

# A model dielectric function with improved local-field effects

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A model dielectric function is developed using the Levine-Louie model dielectric function for insulators, but including microscopic inhomogeneity effects because of the crystal lattice in a manner different from that of Hybertsen and Louie. The model is forced to have the correct macroscopic and high-spatial-frequency static behavior, as well as  $f$ -sum for every matrix element of the dielectric matrix,  $\epsilon_{\mathbf{G}\mathbf{G}'}(\mathbf{q})$ , where  $\mathbf{q}$  is a crystal momentum, and  $\mathbf{G}$  and  $\mathbf{G}'$  are reciprocal-lattice vectors. In real space, this leads to a physically appealing picture of dielectric screening, which involves currents being induced in each region because of local electric fields. Also, the  $\mathbf{G}=0$  row and  $\mathbf{G}'=0$  column of  $\epsilon_{\mathbf{G}\mathbf{G}'}(\mathbf{q})$  have the correct behavior that involves the inner product of  $\mathbf{q}$  and another vector for small  $\mathbf{q}$ . Finally, the correct behavior is achieved in certain, limiting-case model problems, such as the problem of a test charge that is placed within a large void inside of an otherwise uniform dielectric. A realistic test compares the model and random-phase approximation screening of a core hole in a solid.