

Abstract Submitted
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Iterative computation of dielectric eigenmodes HUGH WILSON, FRANCOIS GYGI, GIULIA GALLI, University of California, Davis — We present an iterative method for the calculation of the eigenvectors of dielectric matrices of materials and nanostructures, based on Density Functional Theory, within a linear response framework. We show that by computing a relatively small number of eigenvectors via iterative dielectric response calculations, one may reconstruct the full dielectric matrix of a given system to high accuracy. The proposed method bypasses the need for the calculation of a large number of excited states required by earlier dielectric matrix computations based on the Random Phase Approximation. The scaling of the algorithm and the efficiency of the approach will be demonstrated by the calculation of the static dielectric properties of a variety of nanostructures, including silicon rods and slabs.

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