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Microscopic charge fluctuations in hexagonal boron nitride¹ ADELA NICOLAEV, University of Bucharest, Faculty of Physics, Materials and Devices for Electronics and Optoelectronics Research Center, CLAUDIA RODL, GIULIA PEGOLOTTI, RALF HAMBACH, LUCIA REINING, Laboratoire des Solides Irradies, UMR 7642, CNRS-CEA, Ecole Polytechnique, F-91128 Palaiseau, France and European Theoretical Spectroscopy Facility, STEFAN ANTOHE, University of Bucharest, Faculty of Physics, Materials and Devices for Electronics and Optoelectronics Research Center — We present an ab initio approach to the electron dynamics through the calculation of the total polarizability matrix, including the off-diagonal elements. The charge density induced in a system by an external perturbation is computed in real space and time, following the idea of Abbamonte et al. The difference between our approach and the one from Ref. [1] is that we can calculate not only the diagonal response $\chi(q,q,\omega)$, but also the off-diagonal elements of the matrix $\chi(q,q',\omega)$. Hence, we have access to the microscopic charge oscillations which are induced by the local-field effects. We have studied these charge oscillations at various frequencies comprising interband-transition and plasmon-excitation energies. The real-space approach allows us to see which electrons (or orbitals) contribute to which kind of excitation. The final goal is to offer theoretical support and benchmark to future inelastic x-ray scattering experiments that may measure also the off-diagonal elements of the polarizability. The method is applied to hexagonal boron nitride (h-BN) which is the most stable of the three existing structures (hexagonal, cubic, and wurtzite) at room temperature and ambient pressure.

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