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Density Functional Perturbation Theory on a real space grid[1]
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— The real space implementation of the density functional perturbation theory is reported in which the quantities of interest are defined on a uniform grid, the kinetic energy operator is computed using a high-order finite-difference formula and first principles pseudopotentials are used for the ion-electron interaction. The linear response is obtained on the real space grid. It is applied to calculation of vibrational frequencies and polarizabilities of localized molecular systems, and it is straightforward to use the response in other physical quantities.

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