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Electrical Response of Molecular Chains from Density Functional Theory STEPHAN KUEMMEL, Max-Planck-Institut für Physik Komplexer Systeme, Nöthnitzer Strasse 38, D-01187 Dresden, Germany, LEEOR KRONIK, Department of Materials and Interfaces, Weizmann Institute of Science, Rehovoth 76100, Israel, JOHN P. PERDEW, Department of Physics and Quantum Theory Group, Tulane University, New Orleans, Louisiana 70118, USA — The electrical response of molecular chains is dramatically overestimated by local and semilocal density functionals. We show that Kohn-Sham density-functional theory yields accurate linear and nonlinear polarizabilities when the exact exchange energy is employed together with the corresponding exact Kohn-Sham potential. We further show that approximations to the exact-exchange Kohn-Sham potential that are very accurate for the ground-state energy can nevertheless fail badly for the response because of potential barriers that have little effect on the ground-state energy but strongly affect the electron mobility.

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