Abstract Submitted
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Electron scattering from large molecules: a 3d finite element R-matrix approach[1] STEFANO TONZANI, JILA and Department of Chemistry, University of Colorado, Boulder, CHRIS H. GREENE, Department of Physics and JILA, University of Colorado, Boulder — To solve the Schrödinger equation for scattering of a low energy electron from a molecule, we present a three-dimensional finite element R-matrix method [S. Tonzani and C. H. Greene, J. Chem. Phys. **122** 01411, (2005)]. Using the static exchange and local density approximations, we can use directly the molecular potentials extracted from ab initio codes (GAUSSIAN 98 in the work described here). A local polarization potential based on density functional theory [F. A. Gianturco and A. Rodriguez-Ruiz, Phys. Rev. A **47**, 1075 (1993)] approximately describes the long range attraction to the molecular target induced by the scattering electron without adjustable parameters. We have used this approach successfully in calculations of cross sections for small and medium sized molecules (like SF6, XeF6, C60 and Uracil). This method will be useful to treat the electron-induced dynamics of extended molecular systems, possibly of biological interest, where oth er more complex ab initio methods are difficult to apply.

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