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3d R-matrix calculations of electron scattering from extended molecular systems STEFANO TONZANI, JILA- University of Colorado at Boulder, Boulder, CO 80309-0440, CHRIS H. GREENE, Department of Physics and JILA- University of Colorado at Boulder, Boulder, CO 80309-0440 — We have implemented a three-dimensional finite element approach [S. Tonzani and C.H. Greene, J. Chem. Phys. 014111 **122**, (2005)], to solve the Schrödinger equation for scattering of a low energy electron from a molecule. The potential is treated as a sum of three terms: electrostatic, exchange and polarization. The electrostatic term can be extracted directly from ab initio codes (GAUSSIAN 98 in the work described here), while the exchange term is approximated as a local density functional. 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 very useful to treat the electron-induced dynamics of larger molecular systems, possibly of biological interest, difficult to tackle with more complex ab initio methods. This work has been supported by DOE-Office of Science and NERSC.

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