LOW ENERGY ELECTRON SCATTERING FROM LARGE MOLECULES

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To describe the scattering of a low energy electron from a general polyatomic molecular target, we have implemented a three-dimensional finite element approach [1] in the framework of the R-matrix method. 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 [2] is then constructed in order to describe 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 SF_6, XeF_6, C_{60}, Uracil and other DNA bases)[3].

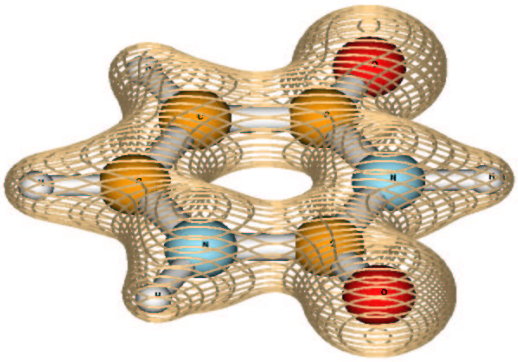

Fig. 1. Electron density and structure of the uracil ground state that we used as a target in our scattering calculations.

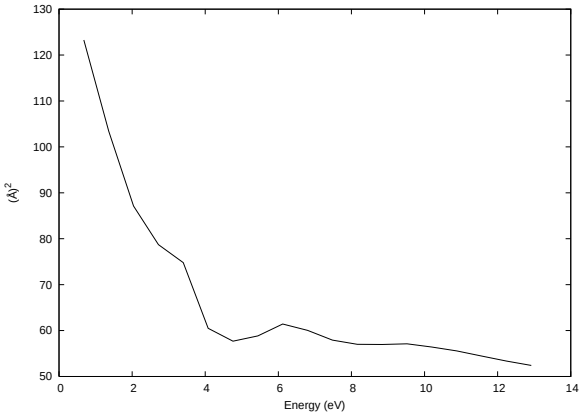

Fig. 2. Elastic cross section for electron scattering from Uracil, preliminary results.

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.
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References

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[2] F. A. Gianturco and A. Rodriguez-Ruiz , Phys. Rev. A **47**, 1075 (1993).

[3] S. Tonzani and C. H. Greene, unpublished (2005).