

RECENT PROGRESS WITH THE SCHWINGER MULTICHANNEL METHOD

Carl Winstead, Vincent McKoy, and Sergio d'A. Sanchez*

A. A. Noyes Laboratory of Chemical Physics, California Institute of Technology, Pasadena, California 91125, USA

*Permanent address: Instituto de Física Gleb Wataghin, Universidade Estadual de Campinas, 13083-970, Campinas, São Paulo, Brazil

When *ab initio* methods for studying electron–molecule collisions were developed, both experiment and theoretical studies were focused on small molecules such as N₂. Although small-molecule studies continue to be important, interest in recent years has increasingly shifted to electron interactions with larger polyatomics. Practical applications within the semiconductor industry, for example, demand electron collision data for molecules such as C₂F₆ or *c*-C₅F₈ [1]. An especially significant development in recent years has been the realization that slow electrons can directly damage DNA [2], which has spurred tremendous interest in low-energy collisions of electrons with DNA bases, sugars, and other biological molecules.

Owing to the low symmetry and the inherent many-electron nature of the problem, accurate calculations of low-energy electron–molecule collisions are computationally demanding. Moreover, as we will emphasize in this talk, the computational requirements scale rapidly with the molecular size, making studies of polyatomic targets especially challenging. To pursue such studies, we have adapted our computational procedure, known as the Schwinger multichannel method, to run efficiently on highly parallel computers, including workstation clusters, and we have made improvements to remove serial bottlenecks, decrease disk usage, and otherwise improve the overall scalability.

In this talk, we will present some of our recent results for elastic and inelastic collisions of low-energy electrons with biological molecules, in particular the DNA bases and the RNA base uracil. Special emphasis will be given to the characterization of low-energy resonances observed in gas-phase scattering [3] and dissociative attachment [4] studies. The assignment of these resonances is still a topic of discussion [5, 6], and by helping to clarify the assignments, theoretical studies may help to clarify the dissociation mechanisms.

Work by C. W. and V. M. was supported by the U. S. Department of Energy, Office of Basic Energy Sciences, and by the U. S. National Science Foundation, Office of International Science and Engineering. S. d'A. S. acknowledges financial support by the Brazilian agencies FAPESP, CNPq, and CAPES.

References

- [1] C. Winstead and V. McKoy, in *Fundamentals of Plasma Chemistry*, M. Inokuti, editor (Adv. At., Mol., Opt. Phys. **43**), 111 (2000).
- [2] B. Boudaïffa, P. Cloutier, D. Hunting, M. A. Huels, and L. Sanche, *Science* **287**, 5458 (2000).
- [3] K. Afatooni, G. A. Gallup, and P. D. Burrow, *J. Phys. Chem. A* **102**, 6205 (1998).
- [4] See, e.g., M. A. Huels, I. Hahndorf, E. Illenberger, and L. Sanche, *J. Chem. Phys.* **108**, 1309 (1998); G. Hanel, B. Gstir, S. Denifl, P. Scheier, M. Probst, B. Farizon, M. Farizon, E. Illenberger, and T. D. Märk, *Phys. Rev. Lett.* **90**, 188104 (2003); R. Abouaf, J. Pommier, and H. Dunet, *Int. J. Mass Spectrom.* **226**, 397 (2003); S. Denifl, S. Ptasinska, M. Cingel, S. Matejcek, P. Scheier, and T. D. Märk, *Chem. Phys. Lett.* **377**, 74 (2003); S. Feil, K. Gluch, S. Matt-Leubner, P. Scheier, J. Limtrakul, M. Probst, H. Deutsch, K. Becker, A. Stamatovic, and T. D. Märk, *J. Phys. B* **37**, 3013 (2004).
- [5] A. M. Scheer, K. Afatooni, G. A. Gallup, and P. D. Burrow, *Phys. Rev. Lett.* **92**, 068102 (2004).
- [6] F. Martin, P. D. Burrow, Z. Cai, P. Cloutier, D. Hunting, and L. Sanche, *Phys. Rev. Lett.* **93**, 068101 (2004).