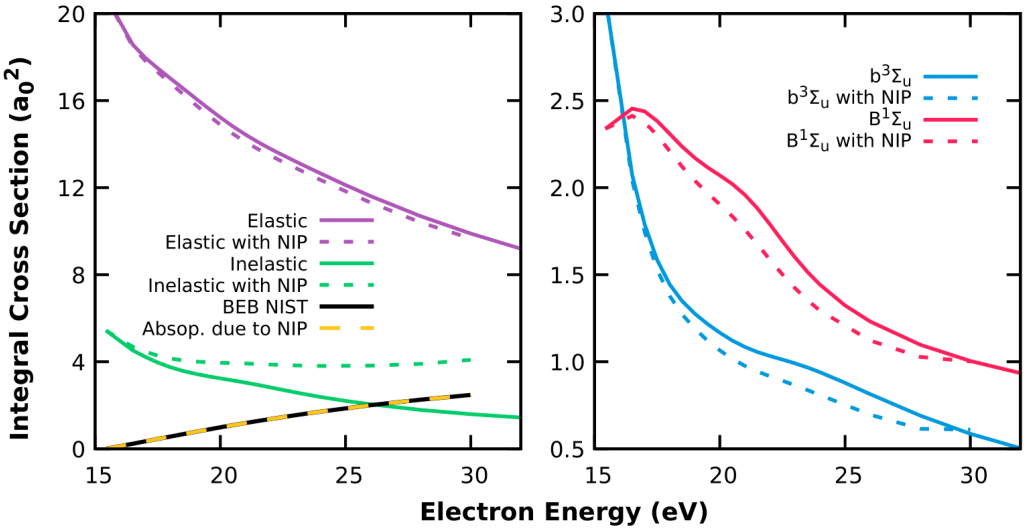
# An iterative negative imaginary potential applied to the Schwinger multichannel method to model ionization effects

A. G. Falkowski[1*], M. H. F. Bettega[2], R. F. da Costa[3], F. Kossoski[4], M. A. P. Lima[1]

[1]*IFGW, Universidade Estadual de Campinas, Campinas, Brazil*
[2]*Departamento de Física, Universidade Federal do Paraná, Curitiba, Brazil*
[3]*Centro de Ciências Naturais e Humanas, Universidade Federal do ABC, Brazil*
[4]*LCPQ (UMR 5626), Université de Toulouse, CNRS, UPS, France*

*email: agf18@ifi.unicamp.br

The Schwinger multichannel method (SMC) [1] is a variational method for the scattering amplitude for electron-molecule collisions. However, only the elastic and electronic excitation channels (involving transitions between bound states) could be addressed within the SMC method. The continuum channels play an important role as the electron impact energy increases (above the ionization threshold). To work around this limitation, we implemented a negative imaginary potential (NIP) to act as a sinkhole of probability flux, where the real part is the electron-molecule interaction potential and the imaginary is the model potential for ionization, as suggested in Ref. [2]. The model potential is a single Gaussian function, parameterized in order to fit the total ionization cross sections (TICS) as obtained with the Binary-Encounter-Bethe (BEB) model [3]. We applied this new technique to investigate the electron scattering by $H_2$ molecules at the multichannel coupling level of three channels (excitation to the first triplet and singlet states, as well as the ground state). Preliminary results are encouraging since we observe a drop in the magnitude of the cross sections due to the presence of the NIP. This feature stimulates the study of the effect of this strategy on multichannel calculations for larger molecules.




**References**

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