Computational Atomic and Molecular Science

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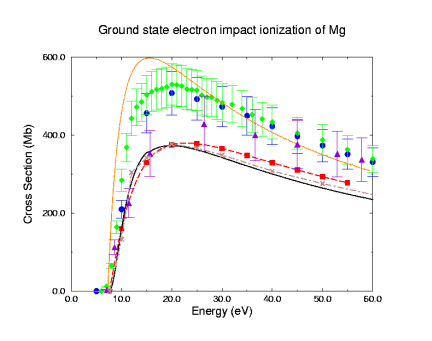
Controlled Fusion Experiments and Astrophysics

Non-perturbative calculations for ionization of inert gases and alkaline earths are required for accurate collisional radiative modeling of astrophysical and tokamak plasmas.

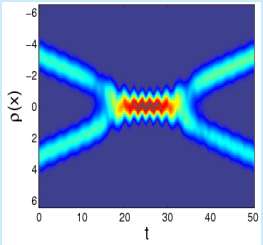


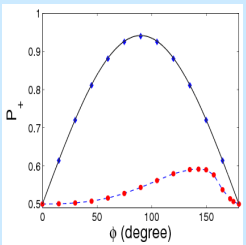
J A Ludlow et al,
Phys. Rev. A 79, 032715 (2009)

Future electron-impact collision calculations using the R-matrix method are expected to use in excess of 50,000 processors for ionization of Mo^+ or excitation of near neutral stages of W

Bose-Einstein Condensate Experiments

Two Bose-Einstein condensates, initially localized in the left and right trap, respectively, move towards each other and pass through. We simulate this process by solving the full three dimensional non-linear Schrödinger equation.





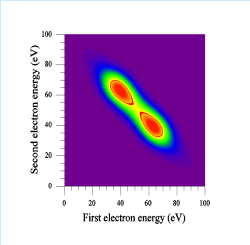
B Sun and M S Pindzola,
J. Phys. B 42, 145502 (2009)

Future multi-species condensate collisions will make use of up to 5000 processors

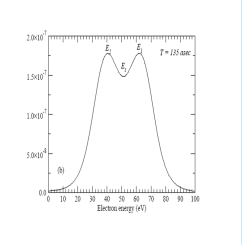
Synchrotron and Laser Experiments

Intense, Attosecond Laser Pulse Double Photoionization of He atom

Probability density of two-photon double ionization. Differential in ejection energies of first electron and second electron.



Single electron energy distribution as a function of ejected energy of one of the electrons.



Teck-Ghee Lee et al,
Phys. Rev. A 79, 053420 (2009)

Future laser pulse and ion-impact scattering from H_2 will make use of up to 50,000 processors