Computational atomic and molecular physics for advances in astrophysics, chemical sciences, and fusion energy sciences

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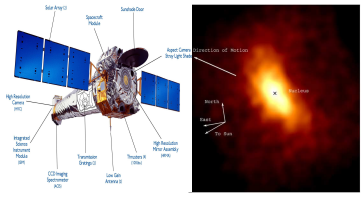
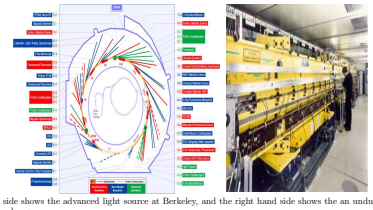
Science Support

Atomic and molecular physics calculations were carried out in support of

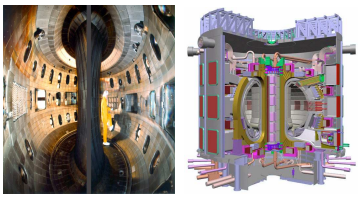
- Astrophysical observations on satellites such as CHANDRA, supported by grants from NASA and PPARC.
- Photon-matter interaction measurements at synchrotron light sources like the ALS, supported by grants from DOE BES.
- Plasma diagnostics on tokamaks like DIII-D and JET, supported by grants from DOE FES.



Left hand side shows a schematic of the CHANDRA X-ray observatory, the right hand side shows an image of the comet C/1999 S4 (LINEAR) that was taken on July 14, 2000.



Left hand side shows the advanced light source at Berkeley, and the right hand side shows the an undulator on the FEL in Hamburg.



Left hand side shows a photograph of the inside of the DIII-D tokamak in California, right hand side shows a schematic of ITER.

Computational Facilities

We use a range of large-scale computing facilities, supported in part by a DOE INCITE award.

- NERSC : IBM-SP3 and IBM-SP5
- ORNL : IBM-SP4 and CRAY-X1E
- PNL : HP-MPP2

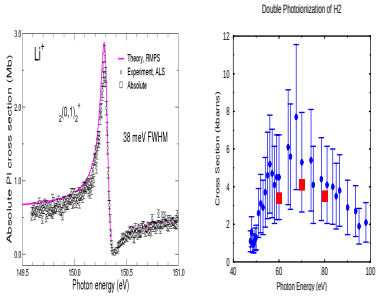
Atomic and Molecular Physics Codes

- Time-dependent close-coupling methods for photon, electron, and atomic ion interactions with atoms and molecules.
- Time-dependent lattice methods for ion-atom collisions and BEC flows.
- R-Matrix for photon and electron interactions with atoms.
- Exterior complex scaling methods for photon and electron interactions with atoms and molecules.
- Perturbative distorted-wave methods for photon and electron interactions with atoms and molecules.
- Classical trajectory Monte Carlo methods for electron and atomic ion interactions with atoms.
- Molecular dynamics simulations for ion-surface interactions.

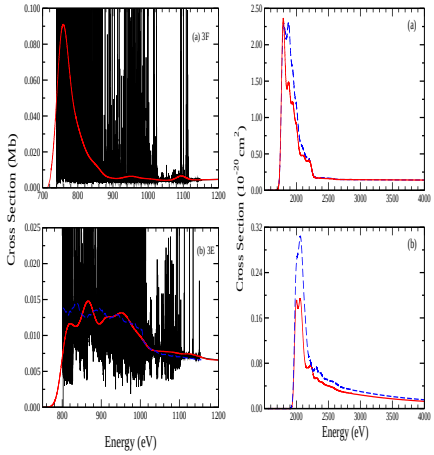
Recent Results

Shown below are a selection of our recent results, including

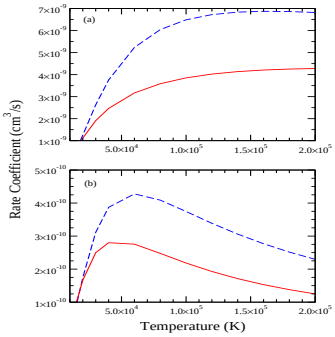
- Photoionization of Li^+ and H_2.
- Electron-impact excitation of He, Fe^{16+} and W^{46+}.
- Electron-impact ionization of C^{2+} and Ar.
- Electron-impact double ionization of H^- and He.
- Heavy particle collisions with He^+ and He.



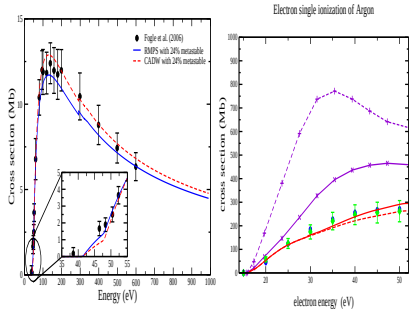
Left hand side shows photoionization of Li^+, right hand side shows double photoionization of H_2.



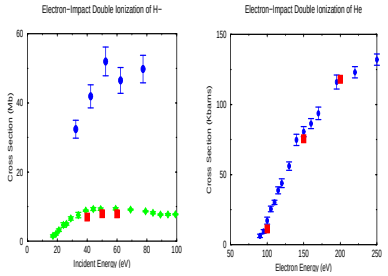
Left hand side shows electron impact cross section for two transitions in Fe^{20+}, right hand side shows a convolved cross section for two transitions in W^{46+}. For the W^{46+} plot the blue line shows the results with no radiation damping, and the red line shows the results with radiation damping included.



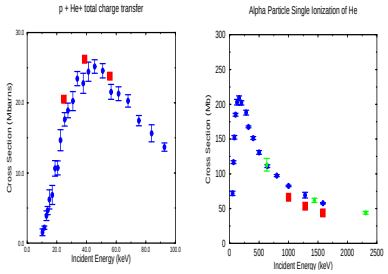
He excitation rate coefficients with and without pseudostates included.



Left hand side shows electron impact ionization cross section of C^{2+}, right hand side shows electron impact ionization of neutral Ar (experiment, RMPS and DW data).



Left hand side shows the electron impact double ionization of H^-, right hand side shows the electron impact double ionizatio of He.



Left hand side shows the proton impact charge transfer with He, the right hand side shows the alpha particle single ionization of He.