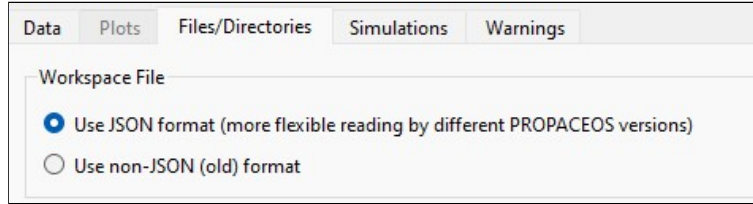




Revisions for PrOpacEOS 11.0.0

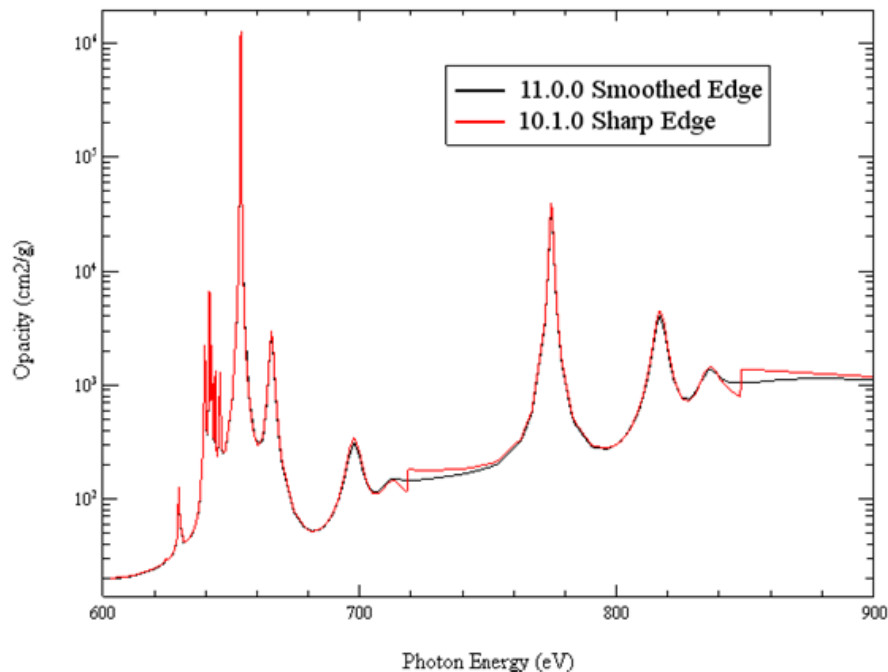
- Support for utilizing JSON-formatted workspaces has been added.
 - This option provides better support for reading/writing workspaces that use different versions of *PROPACEOS*.
 - JSON-formatted files can be readily modified using scripting tools such as Python.
 - To turn this option off, check the "Use non-JSON format" button on the *Directories/Files* tab of *Preferences*. By default, this option is now turned on.
 - When saving a workspace that was originally read in using the old (non-JSON) format, a warning is presented notifying the user that it is now being saved to a JSON-formatted file. (This warning can be turned on/off in the *Warnings* tab of *Preferences*.)



- The OpenGL graphics in each of *PROPACEOS* graphics widgets has been updated to utilize virtual buffer objects. This was done in order for *PROPACEOS* to work effectively on more modern computer monitors and graphics acceleration hardware.
- Derivative quantities dP/dT , dP/dN , and specific heats, for both ions and electrons, are now available for plotting.
- Photoionization edge smoothing. With continuum lowering, the photoionization edge is shifted lower relative to the isolated atom values. This shift is sometimes called ionization potential depression, or IPD. However, experimental results have shown the edges are also likely to have a smooth and round edge, rather than a sharp step used in previous versions of the code. In this release, we have implemented a smoothing procedure for photoionization cross sections. The procedure involves two steps. First the photoionization cross sections of an isolated atom is extrapolated toward the depressed ionization threshold in the log-log scale, and extended further below the threshold at a constant value. We then determine the multiplicative smoothing factor

$$S(E, E_{th}) = \int_{-\infty}^E \phi(E', E_{th}, w) dE'$$

where $\phi(E, E_{th}, w)$ is the Stark line profile for a bound-bound transition close in energy to the depressed ionization threshold E_{th} with corresponding broadening FWHM w . The product of this factor and the extrapolated photoionization cross section provide the smoothed absorption edges. An example of the smoothing is shown below for the opacities of He-like and H-like Oxygen ions.



- Extending maximum number of levels in atomic models. Previous versions of atomic model file (atm) file format had a hard limit on the maximum number of levels. This new release removes this limitation. The formats of several input (atm file) files have been extended such that data columns involving level and transition indices now have a larger width to avoid overflow. As a result, the new atm files cannot be read by older versions of *AtomicModelBuilder*, *PrismSPECT*, *PROPACEOS*, and *Spect3D*.
- Bug fixes:
 - Previously, when plotting results, the mass conversion for plots of density was incorrect for isotopes (e.g., D and T). This has been fixed, so the conversion to g/cc is now correct.
 - Previously, when using the -z option, the simulation was run as non-DCA. This has been fixed.
 - Previously, the warning "It is recommended to use a max photon energy of at least 10x the max temperature" could improperly appear when tabulated photon energies and/or tabulated temperatures were used. This has been fixed.
 - Convergence improvement of steady state block matrix solver. *PROPACEOS* 10.1.0 introduced a block matrix solver for NLTE steady state solution to handle larger atomic systems more efficiently. The solver was found to occasionally fail for complex atomic systems. *PROPACEOS* 11.0.0 includes improvements to the stability of the solver.
 - Improvement to photon energy grid construction method. Previous versions may fail for large atomic models when number of transitions are very large, such that resolving bound-bound transitions with sufficient accuracy requires number of photon energy points to exceed the preset limit. *PROPACEOS* 11.0.0 implements an iterative procedure to relax the resolution requirement such that the total number of photon energy points always stay close to the preset limit.