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Extending and Smoothing Two-dimension Equation of State Simulation Data

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Disclaimer

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ABSTRACT

The Multiphase Equation of State (MEOS) project works to produce high quality equation of state tables which are used in computationally intensive simulations of materials in different conditions. An equation of state table describes the state of matter under certain physical conditions such as pressure, volume, temperature, or internal energy. MEOS uses many different models and combinations thereof to produce accurate tables consisting of continuous smooth data, derivatives, and higher-order derivatives. Accurate and smooth data are important factors in producing precise simulations. This report focuses on improving the electron tables produced from Purgatorio and Thomas-Fermi data. Purgatorio data is extremely accurate but often jagged and discontinuous in the lower temperature and density region. Thomas-Fermi is a model that provides smooth data throughout. Together, this produces an EOS data table that is both accurate and smooth. This report describes the implementation of a new feature that allows users to define more detailed regions in the Purgatorio table to be replaced with Thomas-Fermi. As a result, MEOS can generate a table that is both more smooth and still accurate.

INTRODUCTION

Solids, liquids, gases, and other such phases, interact with one another every moment. The results of these interactions are important in many applications. Scientists simulate these interactions within stars, nuclear fusion, atmospheres, etc.

Equation of state (EOS) data tables are heavily utilized in these simulations. EOS is a thermodynamic equation used to describe the state of a matter under certain physical conditions such as pressure, volume, temperature, or internal energy. This allows an accurate description of phase changes, or in other words, the transformation of solids to liquids or other such phases.

To provide useful EOS data tables, the data must be both accurate and smooth. This is because of the several variables calculated by MEOS. The pressure and entropy variables are calculated from the density and temperature derivatives of the free energy variable. Other variables, such as energy or sound speed, are then calculated from pressure and entropy. For this reason, simulations require both accuracy and smoothness, so that derivatives and higher-order derivatives are also accurate.

Due to the importance of EOS tables, many different projects were developed to assist in creating them. One of these projects is called the Multiphase Equation of State (MEOS). MEOS utilizes many different models and combinations thereof to produce EOS data tables.

This report focuses on the 2-dimensional table in MEOS used to calculate the electron free energy term. There are multiple ways to produce this type of table. The most common way is by combining two different tables: Purgatorio and Thomas-Fermi.

Purgatorio is the improved Inferno algorithm. It uses the averaged-atom-in-jellium approximation to provide highly accurate data. Essentially, the data is computed by treating the atoms as if they were spherical and embedded in an electron gas called jellium. It is widely recognized as a very good model. Unfortunately, the data becomes jagged and discontinuous in the lower temperature and density region. MEOS strives to provide data that is accurate and smooth across a range of different conditions.

As a result, Thomas-Fermi data is combined with Purgatorio. This data utilizes both classical and quantum mechanics to express the electron-thermal free energy. This table was widely used before the introduction of Purgatorio. It was a basic model that allowed extrapolation from hydrogen to other elements once the data was computed. Due to its nature, Thomas-Fermi

omits key details in quantum and relativistic effects. Consequently, its data is not as accurate as Purgatorio, but it is extremely smooth.

MEOS allowed users to combine these tables together through a simple cutting and attaching process modeled by PurgaExtendWithTF, PurgaExtendWithTF2, and PurgaExtendWithTF3. This report focuses on the implementation of PurgaExtendWithTF4, which allows a more sophisticated manner of defining the Thomas-Fermi extension.

MEOS ELECTRON TABLES

MEOS is used by inputting a file with the type and characteristics of the model being used. When using the PurgaExtendWithTF models, the user may define markers. Markers define the regions on the table for which the Thomas-Fermi data replaces the Purgatorio data. The models then utilize a transition algorithm to ensure smoothness around the transition points.

The tables below demonstrate the need to replace certain regions in the Purgatorio table with the smooth data from the Thomas-Fermi table.

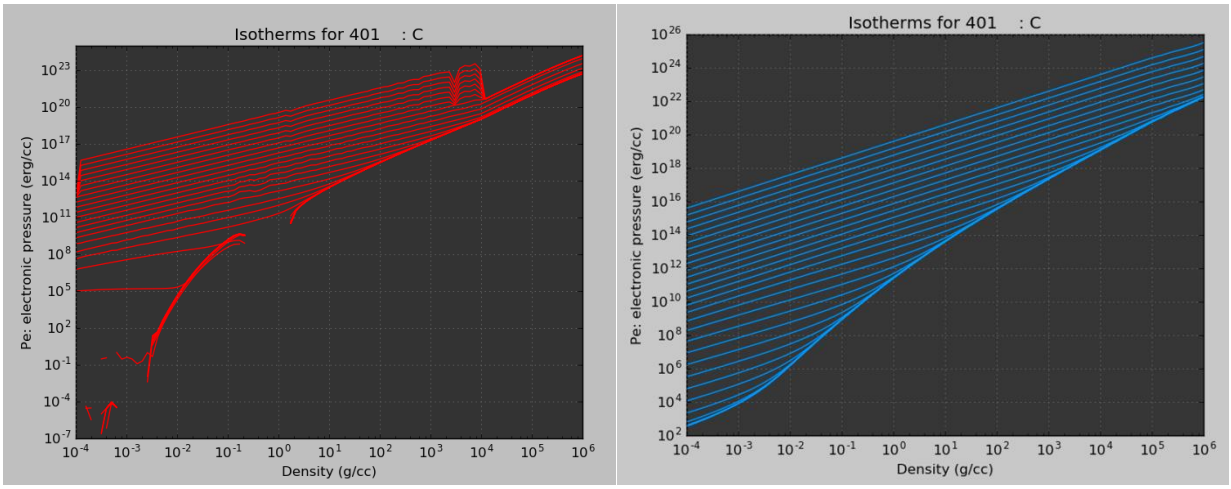

Fig. 1. The left graph in red is the isotherm graph for Carbon produced by Purgatorio data. The right graph in blue is the isotherm graph for Carbon produced by Thomas-Fermi data.

Markers

There are multiple types of markers available in MEOS. Due to its convenience for the user, the straight-lined Threshold Marker is used. This sort of marker is easy for the user to understand and modify. Throughout this report, markers will be written using inequalities and an axis character (ex. >5t: greater than 5 Kelvin, >5r: greater than 5 g/cc).

In PurgaExtendWithTF and PurgaExtendWithTF2, MEOS allowed users to define a density point. Anything below that point used Thomas-Fermi data, while anything above was Purgatorio. PurgaExtendWithTF3 improved upon this by allowing multiple markers on either the temperature or density axis.

An example of PurgaExtendWithTF3 using two markers can be seen below.

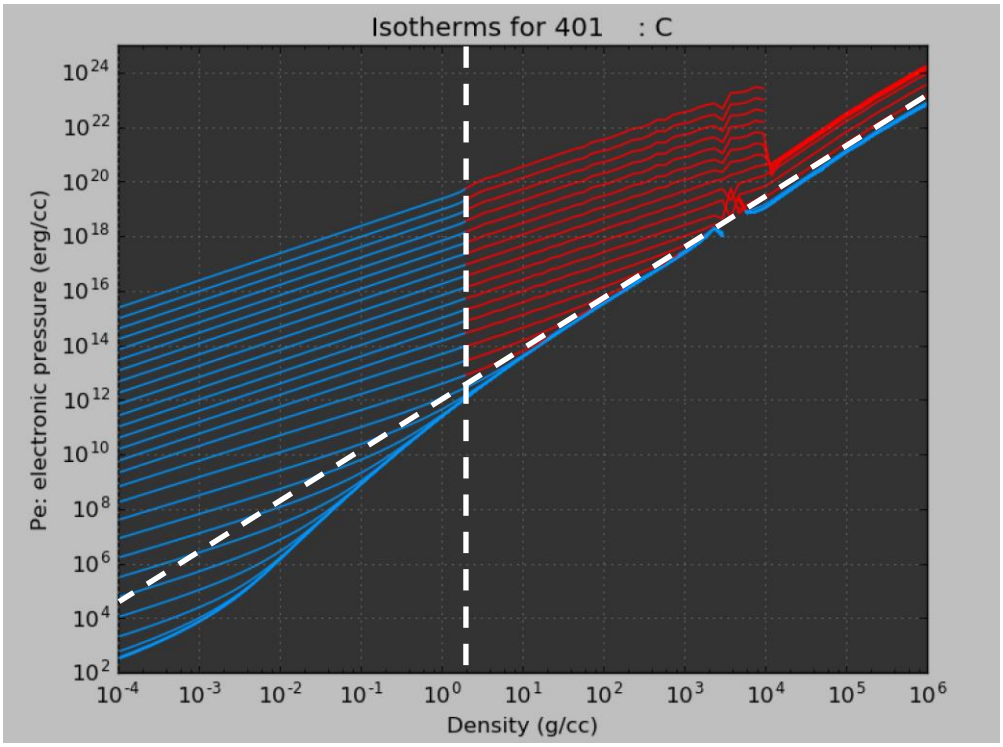

Fig. 2. The isotherm graph for Carbon produced by the PurgaExtendWithTF3 model using the marker: [<2r, <2e7t]. The region less than 2 g/cc or less than 2×10^7 Kelvin utilizes Thomas-Fermi data in blue. The remaining region in red utilizes Purgatorio data. The marker is shown on the graph by the white dashed line.

Extending Purgatorio with Thomas-Fermi

MEOS produces the combined Purgatorio and Thomas-Fermi table by starting off with the Purgatorio data. In the first two versions of the model, MEOS simply replaces anything below the density transition point with Thomas-Fermi data. In PurgaExtendWithTF3, the algorithm iterates through the list of markers. For example, if the markers are defined as [<2r, <2e7t], the algorithm will first incorporate the Thomas-Fermi data in the region less than 2 g/cc. It will then incorporate the Thomas-Fermi data in the second region less than 1000 Kelvin.

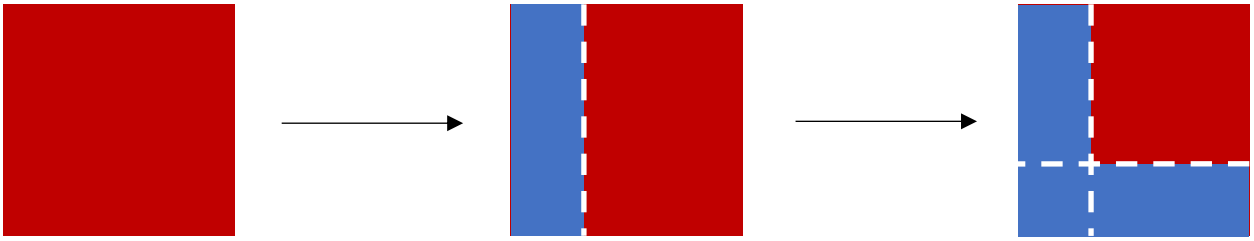

Fig. 4. The red Purgatorio table is iteratively replaced by the Thomas-Fermi data as the algorithm goes through the markers.

Transition between Purgatorio and Thomas-Fermi

Simply inserting Thomas-Fermi data into a Purgatorio table will not ensure smoothness. Realistically, the jaggedness that the Thomas-Fermi data was attempting to fix would be introduced at the marker line. As a result, the Thomas-Fermi data is adjusted to meet Purgatorio at the transition point. This is because users utilize Purgatorio mainly for its accuracy and Thomas-Fermi mainly for its smoothness. Since the algorithm implements each marker independently, the Thomas-Fermi data is adjusted to meet the Purgatorio data at the transition for the marker being implemented.

Thomas-Fermi data (*TFCurrent*) is adjusted by using the value of the Thomas-Fermi table at the transition point (*TFTransition*) and the value of the Purgatorio table also at the transition point (*PurgaTransition*). The algorithm adjusts the relative relation between *TFCurrent* and *TFTransition* to that of the *PurgaTransition* value, or in other words, $(TFCurrent \div TFTransition) \times PurgaTransition$.

To allow an even smoother transition, points around the marker are not adjusted but deleted altogether. This space is then interpolated through by the Livermore Interpolation Package, or the LIP2DFunction in the MEOS project. The number of points deleted around markers is defined in the input file as the DeletePercentage.

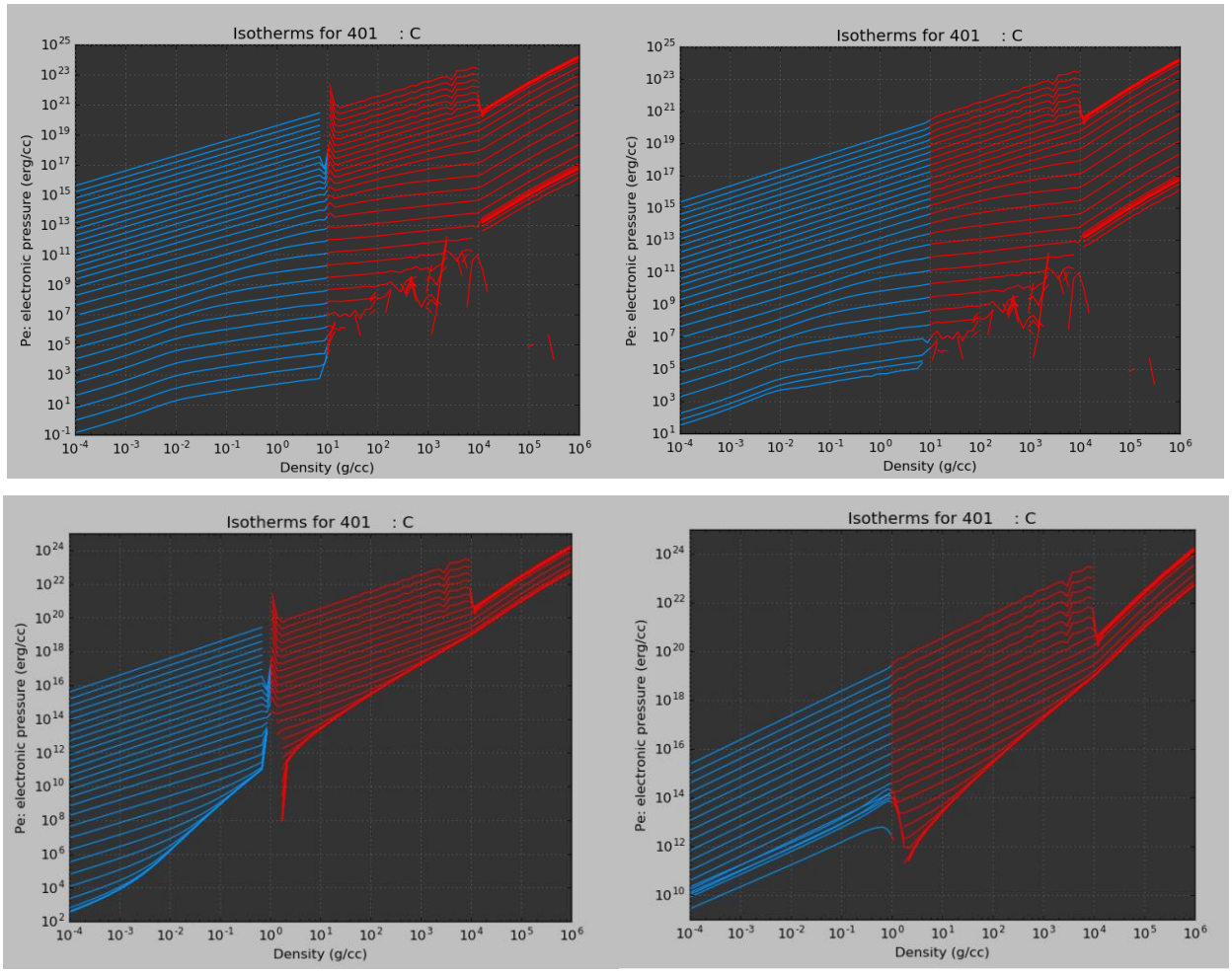

Fig. 6. The left graphs do not implement any transition algorithm between the blue Thomas-Fermi region and the red Purgatorio region at the transition line (10^1 g/cc for the top graphs; 10^0 g/cc for the bottom graphs). The right graphs adjust the Thomas-Fermi data and interpolates across the transition line.

PURGAEXTENDWITHTF4

PurgaExtendWithTF4 improves upon PurgaExtendWithTF3 by allowing more flexibility in defining the Thomas-Fermi regions. PurgaExtendWithTF4 implements a feature that allows users to define several distinct regions. A marker of [[<1t, <50r], [>100t, >200r]] defines two separate regions to be modeled by Thomas-Fermi. The first region is less than 1 Kelvin and less than 50 g/cc. The second region would be greater than 100 Kelvin and greater than 200 g/cc.

An example with several distinct regions can be seen below.

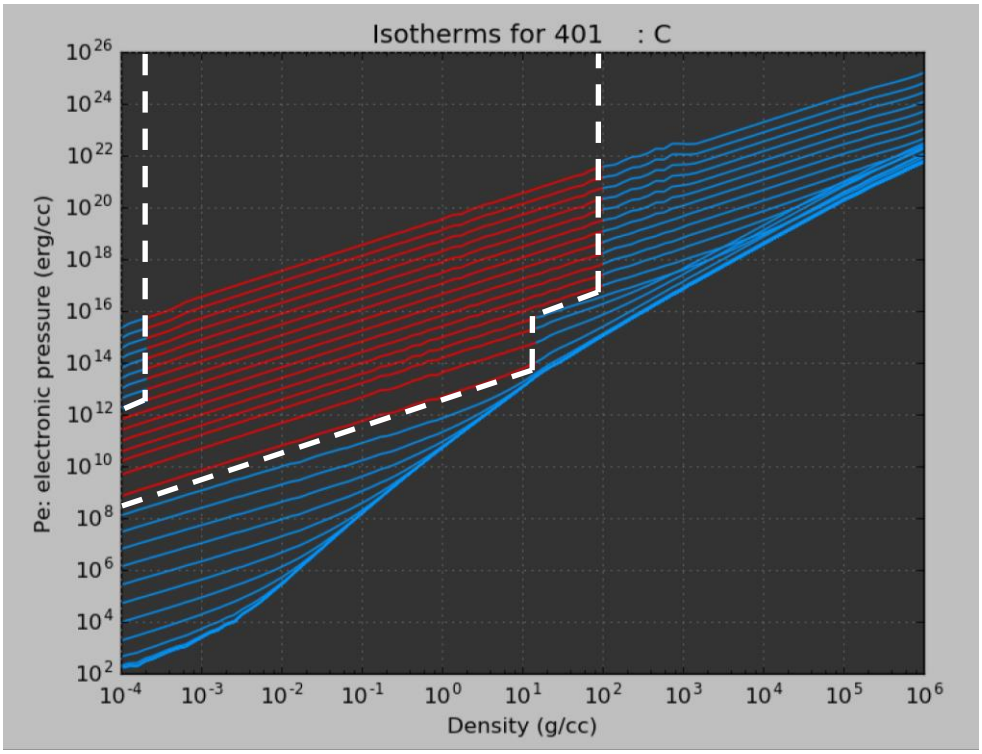

Fig. 3. The isotherm graph for Carbon produced by the PurgaExtendWithTF4 model using the marker: [[<1e6t, <100r], [>20r, <1e8t], [>10e2r], [<5e-4r, >1e9t]]. Regions in blue (top right and bottom left) utilize Thomas-Fermi data. The remaining region in red utilizes Purgatorio data. The marker is shown on the graph in the white dashed line.

The algorithm allows multiple regions by starting off with the Thomas-Fermi table, unlike the previous models. For the first region, the Thomas-Fermi table is replaced by the Purgatorio data for each marker. This means that for a marker such as [<0.5r, <1000t], the resulting first

region will incorporate Thomas-Fermi data in the region that is both less than 0.5 g/cc and less than 1000 Kelvin. This is different from PurgaExtendWithTF3 which would have placed Thomas-Fermi data in any region less than 0.5 g/cc or less than 1000 Kelvin.

To incorporate the second region of Thomas-Fermi in PurgaExtendWithTF4, the table with the first region incorporated is copied. A new Thomas-Fermi table is also generated. The second list of markers is iterated through, and a similar process is applied. The Thomas-Fermi table is replaced by the copied table containing the previous region. This copied table would be mostly Purgatorio except for the one region of Thomas-Fermi. This method allows the first region to be kept while incorporating the second region.

Once this region of Thomas-Fermi is incorporated, a new copy is made, and a new Thomas-Fermi table is generated again to incorporate the next region. This process is repeated until all Thomas-Fermi regions are incorporated.

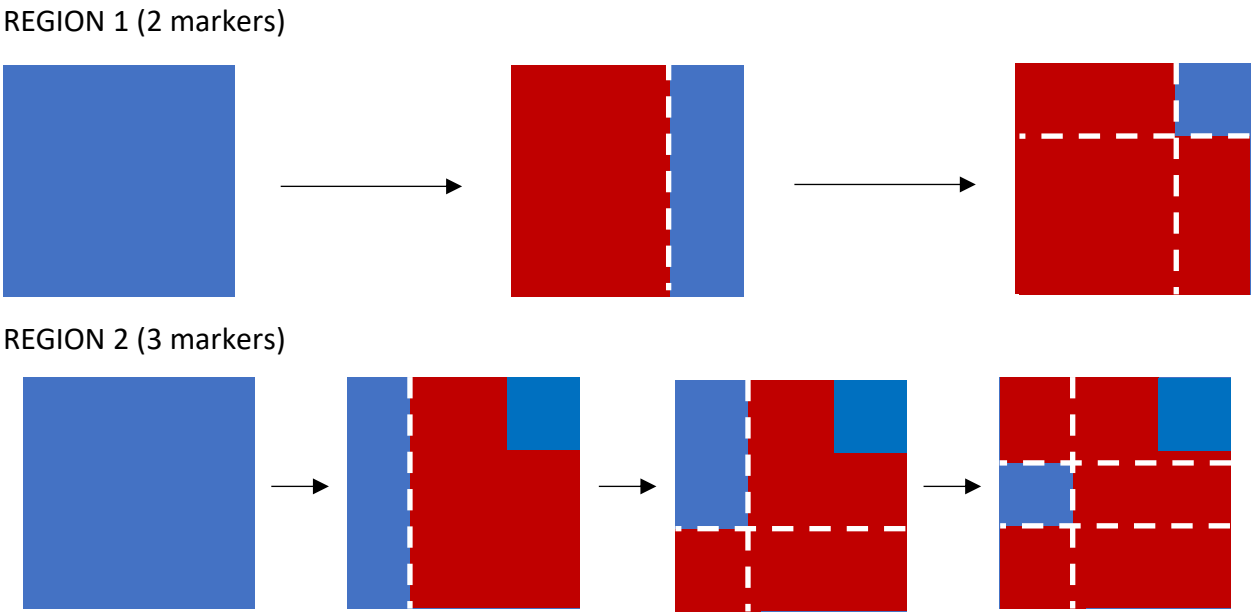

Fig. 5. The blue Thomas-Fermi table is iteratively replaced by the Purgatorio data as the algorithm iterates through the list of markers for the first region. The second region is integrated by having a new Thomas-Fermi table iteratively replaced by the data from the table with the first region incorporated. This process is repeated for all Thomas-Fermi regions.

Transition

PurgaExtendWithTF4 utilizes the same transitioning algorithm as the previous models. Despite starting with Thomas-Fermi data and then inserting Purgatorio data, efforts are still made to only adjust the Thomas-Fermi data. For each marker, the entire data table is repopulated and anything within the marker region that is not Purgatorio is modified to match the previous table, whether that is pure Purgatorio, or Purgatorio with some Thomas-Fermi regions incorporated.

Improvements

PurgaExtendWithTF4 still has room for improvement. Transitions between Purgatorio and Thomas-Fermi can always be smoother and overlapping regions may also cause unwanted behaviors. Other improvements include incorporating different types of markers beyond simple straight lines from a certain axis. This could include functions such as linear or polynomial equations.

Regardless, this new implementation is already beneficial. Users using MEOS to produce electron tables now have more control in combining Purgatorio and Thomas-Fermi. Higher quality EOS data tables can now be produced. This will increase the accuracy of the simulations that utilize such an EOS table and ultimately benefit many projects.

ACKNOWLEDGEMENTS

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REFERENCES

1. B. Wilson, V. Sonnad, P. Sterne, W. Isaacs, "Purgatorio - A new implementation of the Inferno algorithm," *Journal of Quantitative Spectroscopy and Radiative Transmission, vol. 99, no. 1-3, June 1, 2006, pp. 658-679* (2005).
2. Christine J. Wu, Philip C. Myint, John E. Pask, Carrie J. Prisbrey, Alfredo A. Correa, Phanish Suryanarayana, and Joel B. Varley, "Development of a Multiphase Beryllium Equation of State and Physics-based Variations," *The Journal of Physical Chemistry A* (2021).
3. Christine Wu, Philip Myint, Randolph Hood, Miguel Morales-Silva, Lorin Benedict, David Young, John Moriarty, Phil Sterne and Daniel Orlikowski, "Multiphase Equation of State and Melt," *LLNL Physics and Life Sciences Directorate*.
4. Hiromasa Mazaki, "Equations of State of Atoms for the Thomas-Fermi Theory: Applications for Atoms under a High Pressure," *Bulletin of the Institute for Chemical Research, Kyoto University* (1975).