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Atom-in-jellium equations of state for cryogenic liquids[1] TOM LOCKARD, LORIN BENEDICT, PHILIP STERNE, MANDY BETHKENHAGEN, SEBASTIEN HAMEL, DAMIAN SWIFT, Lawrence Livermore Natl Lab
— Modeling the electronic structure of an atom as a homogeneous electron gas or jellium yields a computationally efficient method for calculating the equations of state (EOS) that has been shown to be consistent with the more rigorous methods employing path-integral Monte Carlo and quantum molecular dynamics (QMD) simulations of metals in a warm dense matter regime. Here we apply the atom-in-jellium model to predict wide-ranging EOS for the cryogenic liquid elements nitrogen, oxygen, and fluorine. The principal Hugoniots for these substances were surprisingly consistent with the available shock data and Thomas-Fermi (TF) EOS for very high pressures and exhibited systematic variations from TF associated with shell ionization effects. The new EOS extend much higher in pressure than previous widely-used models for nitrogen and oxygen in particular, and should allow much more accurate EOS to be predicted for oxides and nitrides in the liquid, vapor, and plasma regime, where these have previously been constructed as mixtures containing the older EOS.

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