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Theoretical Equation of State for Beryllium-Oxide[1] JONATHAN BOETTGER, KEVIN HONNELL, Applied Physics Division, Los Alamos National Laboratory — All-electron electronic structure calculations, using two distinct density functional approximations, have been used to predict the zero temperature equation of state and structural phase stability of beryllium-oxide (BeO) up to 1 TPa. A Sesame-type equation of state for BeO has been constructed using the new electronic structure results. The predicted 300 K isotherm and Hugoniot will be compared with experimental data.

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