Abstract Submitted
for the SHOCK15 Meeting of
The American Physical Society

High pressure phase diagram of MgO MARTIN FRENCH, DANIEL CEBULLA, RONALD REDMER, University of Rostock, Institute of Physics — In order to improve the understanding of the interior of super-Earths (planets in the range of 1-10 Earth masses) and other exoplanets, ab inito calculations for the planetary materials and the equation of state (EOS) and phase diagram of planetary materials are needed. A typical representative is MgO, which is an abundant material in the Earth's mantle and is also expected to be important for the mantle of exoplanets as well as for the rocky cores of gas giants such as Jupiter. Using ab initio molecular dynamic simulations, we have determined the phase diagram for MgO up to 20000 K and 1.5 TPa. In particular, the transition from the solid to the molten salt has been studied using diffusion analyses and pair distribution functions. The transition from the B1 to the B2 structure in solid MgO is determined by calculating the respective free enthalpies. The phase diagram of MgO is constructed based on accurate EOS data. We compare with results from (decaying) shock and ramp compression experiments and theoretical calculations for the B1-B2 and the liquid-solid transition line [1, 2, 3].

[1] R.S. McWilliams et al., Science, **338**, 1330 (2012).
[2] F. Coppari et al., Nat. Geoscience, **6**, 926 (2013).
[3] D. Cebulla et al, PRB, **89**, 134107 (2014)

Daniel Cebulla
University of Rostock, Institute of Physics

Date submitted: 03 Feb 2015 Electronic form version 1.4