Ab-initio shock states and thermodynamic properties of liquid silicates

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We present *ab-initio* calculations of the principal Hugoniot states, entropy, sound velocity, as well as transport properties for liquid silicate Mg_2SiO_4. Our investigations heavily employ density functional theory-based molecular dynamics (QMD) calculations to self-consistently compute thermodynamic quantities. In this presentation, we discuss the Hugoniot states and possible de-mixing of liquid Mg_2SiO_4. We then turn to new calculations of entropy on the Hugoniot of Mg_2SiO_4 using the 2PT method [1] and compare to results from more traditional thermodynamic integration. Wherever possible, we compare our results to experiment. The results highlight the utility and predictive power of QMD methods for high energy density physics.

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REFERENCES

[1] M.P. Desjarlais, *"First-principles calculation of entropy for liquid metals"*, PRE **88**, 062145 (2013).