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Equation of State and Viscosity of Tantalum and Iron from First Principles LJUBOMIR MILJACIC, STEVEN DEMERS, AXEL VAN DE WALLE, California Institute of Technology — To understand and model at continuum level the high-energy-density dynamic response in transition metals like Tantalum and Iron, as it arises in hypervelocity impact experiments, an accurate prediction of the underlying thermodynamic and kinetic properties for a range of temperatures and pressures is of critical importance. The relevant time scale of atomic motion in a dense gas, liquid, and solid is accessible with *ab-initio* Molecular Dynamics (MD) simulations. We calculate EoS for Ta and Fe via Thermodynamical Integration in 2D (V,T) phase space throughout different single and two-component phases. To reduce the *ab-initio* demand in selected regions of the space, we fit available gas-liquid data to the Peng-Robinson model [1] and treat the solid phase within the Boxed-quasi-harmonic approximation [2]. In the fluid part of the 2D phase space, we calculate shear viscosity via Green-Kubo relations, as time integration of the stress autocorrelation function.

[1] Ind. Eng. Chem., Fundam **15**, 59 (1976)
[2] A. van de Walle and G. Ceder, *Rev. Mod. Phys.* **74** 11 (2002)

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