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**Structures, properties, and phase Transformations of Ta at high pressures and temperatures** DENNIS KLUG, National Research Council of Canada, YANSUN YAO, University of Saskatchewan, NRC-UNIVERSITY OF SASKATCHEWAN COLLABORATION — High pressure structures and phase transitions of dense Ta were studied with several theoretical methods to address recent controversies regarding the properties of this element. The objective is to characterize the structure of Ta at high temperatures and pressures where possible phase transitions could occur and have been reported. The techniques employed include structure search methods and the metadynamics method based on density functional theory, together with a detailed analysis of the mechanical and dynamical properties of candidate structures that may be stable near the melting temperature of Ta and to pressures up to several TPa which are currently obtainable in shock-compression experiments. This includes a characterization of anharmonic effects on the dynamical and mechanical stability of Ta over the temperature range from 0 K to the melting temperature.

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