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Vibron Dynamics of Hydrogen at High Pressures and Temperatures KARL JOHNSON, University of Pittsburgh, JOSEPH FELDMAN, Center for Computational Materials Science, Naval Research Laboratory, and School of Computational Sciences, George Mason University, RUSSELL HEMLEY, Geophysical Laboratory, Carnegie Institution of Washington — There is currently great interest in the behavior of molecular hydrogen at high pressures and temperatures. The van Kranendonk theory of vibrons in solid hydrogen has been used previously to provide a description of the Raman response as a function of pressure and para-ortho concentrations at low temperature. Here we apply the same model to very different environments, namely to the solid at high P-T conditions, and, with less justification, to the dense fluid. The effect of temperature is presumed to be to renormalize the hopping parameter. Within our model of the vibrons and approximate harmonic lattice dynamics, a $1/R^6$ dependence of the hopping parameter on intermolecular distance, R , gets averaged over fluctuations in the interatomic distance, and the average increases with temperature. Preliminary results using configurations obtained from hybrid path integral molecular dynamics calculations with empirical potentials suggest that there is very little change in the Raman peak upon melting at high pressure, in agreement with previous high P-T measurements.

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