

Second-order many-body perturbation study of Ice-VIII

Kandis Gilliard¹, Olaseni Sode² and So Hirata¹

*¹Department of Chemistry, University of Illinois at Urbana-Champaign
600 South Matthews Avenue, Urbana, Illinois 61801, U.S.A.*

*²Department of Chemistry, University of Chicago
5801 South Ellis Avenue, Chicago, IL 60637*

ABSTRACT

Ice-VIII is a high-pressure polymorph of water Ice. With the use of our embedded-fragmentation method, we have calculated the structures and vibrational spectra of the 3D-Infinite crystal of Ice-VIII at various Pressures with second-order many-body perturbation theory. Our calculations reproduce the structural and vibrational properties of Ice-VIII as well as possibly address the apparent anomalous changes of Ice-VIII at ambient and higher pressures.