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Towards a mulitphase equation of state of Carbon from first principles ALFREDO CORREA, University of California at Berkeley and Lawrence Livermore National Laboratory, LORIN BENEDICT, ERIC SCHWEGLER, Lawrence Livermore National Laboratory — Ab initio molecular dynamics and electronic structure calculation had become one of the most useful tools to investigate properties of materials. Unfortunately these atomistic detailed results are rarely reused in calculations at a higher level of description, such as fluid dynamics and finite elements calculations. In this talk we present a concrete example showing the way that first principles results can be expressed in a way that is useful for hydrodynamics calculations, in particular we show how to build a analytic equation of state for Carbon that involves solid (diamond and BC8) and liquid phases. Applications of this newly obtained equation of state will be presented. This work was performed under the auspices of the U.S. Dept. of Energy at the University of California/Lawrence Livermore National Laboratory under contract no. W-7405-Eng-48.

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