

Equation of State of Water Based on SCAN Meta-GGA Density Functional

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CONVERGENCE OF THE CALCULATED PRESSURE AND ENERGY

Here, we choose three simulation points near the LLT in the 273 K isotherm and present the calculated energy and/or pressure at each point as functions of time steps in Figs. S1 and S2. It can be seen that at the three simulation points, the calculated energy and/or pressure converge, indicating that the system arrives at equilibration.

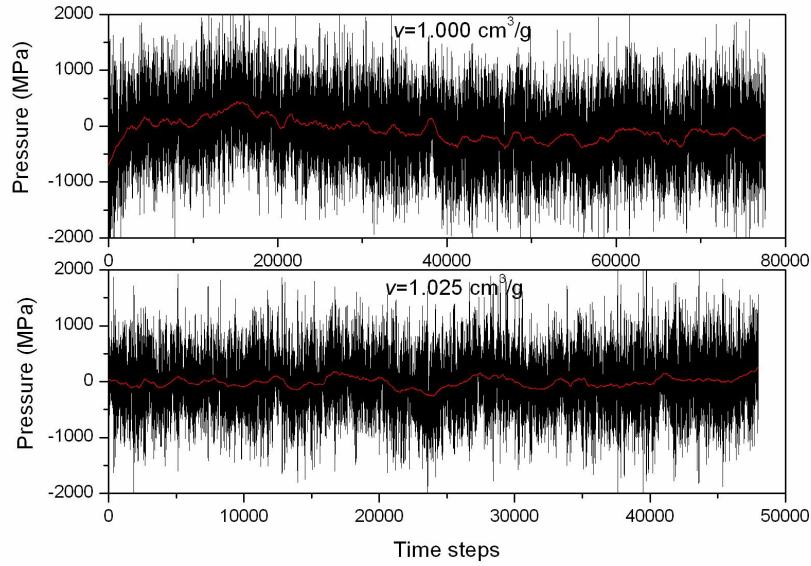


Fig. S1 The calculated pressure as functions of time steps for the 96-atom system. At the two simulation points, the calculated pressure converge after 40000 and 10000 time steps respectively, indicating that the system arrives at equilibration.

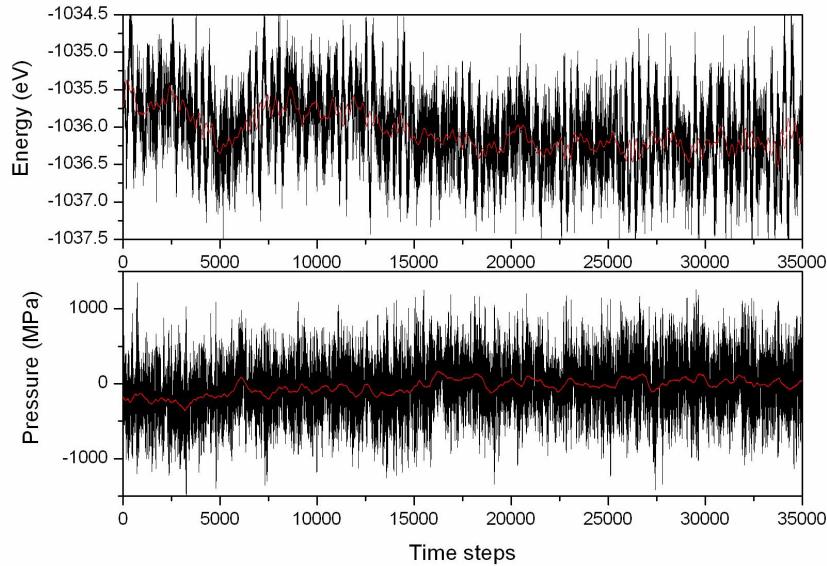


Fig. S2 The calculated energy and pressure as functions of time steps for the 192-atom system at $T = 273$ K and $v = 1.00 \text{ cm}^3/\text{g}$. After 15000 time steps, the system arrives at equilibration.