To the Pore and Through the Pore: Thermodynamics and Kinetics of Helium in Exotic Cubic Carbon Polymorphs

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Number of Figures: 2

Number of Pages: 3

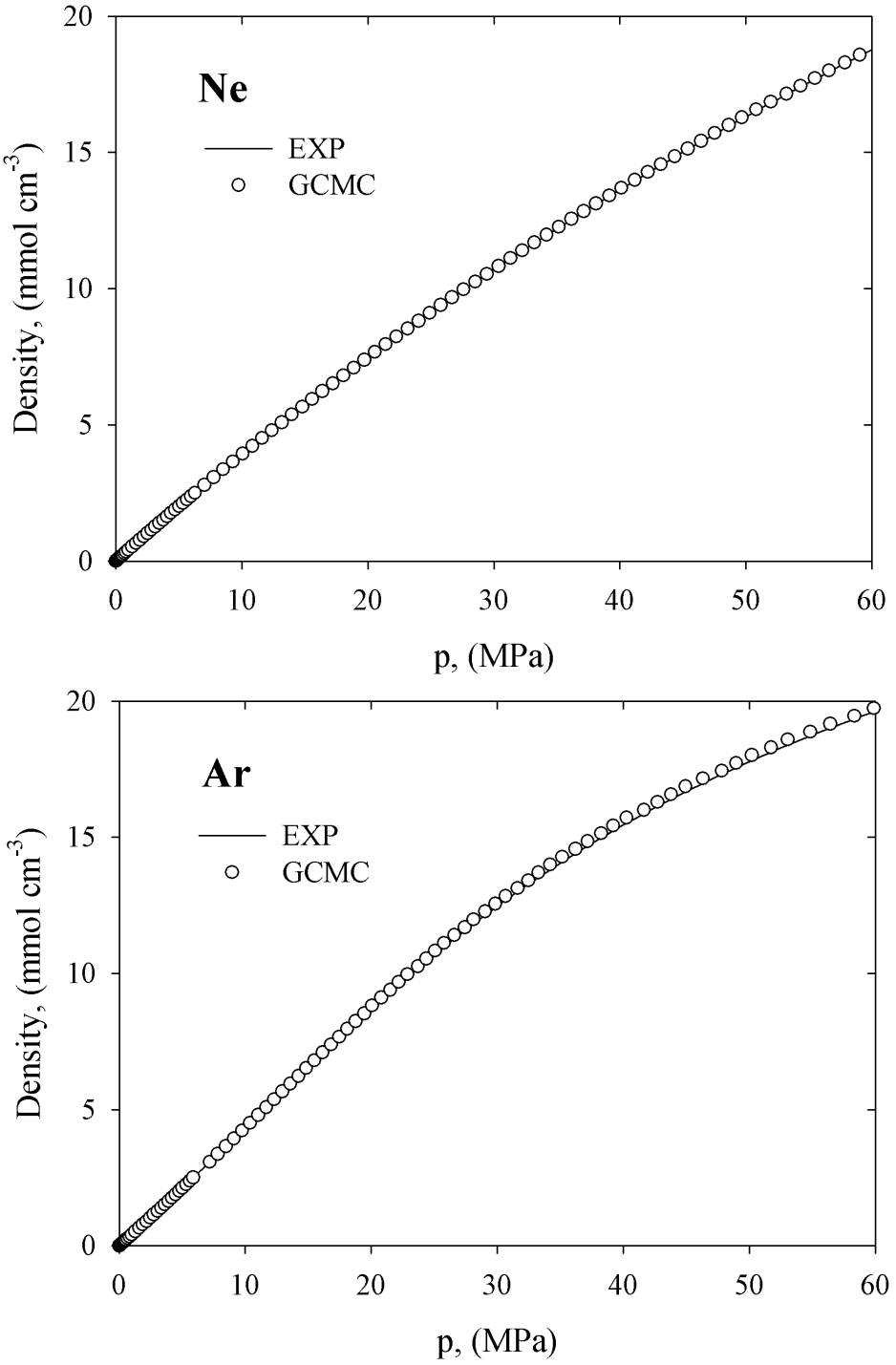

Figure 1S. Comparison of the experimental equation of states for Ne and Ar fluids at 298 K (solid lines)[5] with the ones computed from Monte Carlo simulations in the grand canonical ensemble (open circles). For Ne and He, the (12,6) LJ potential[3] implemented in standard GCMC was used.

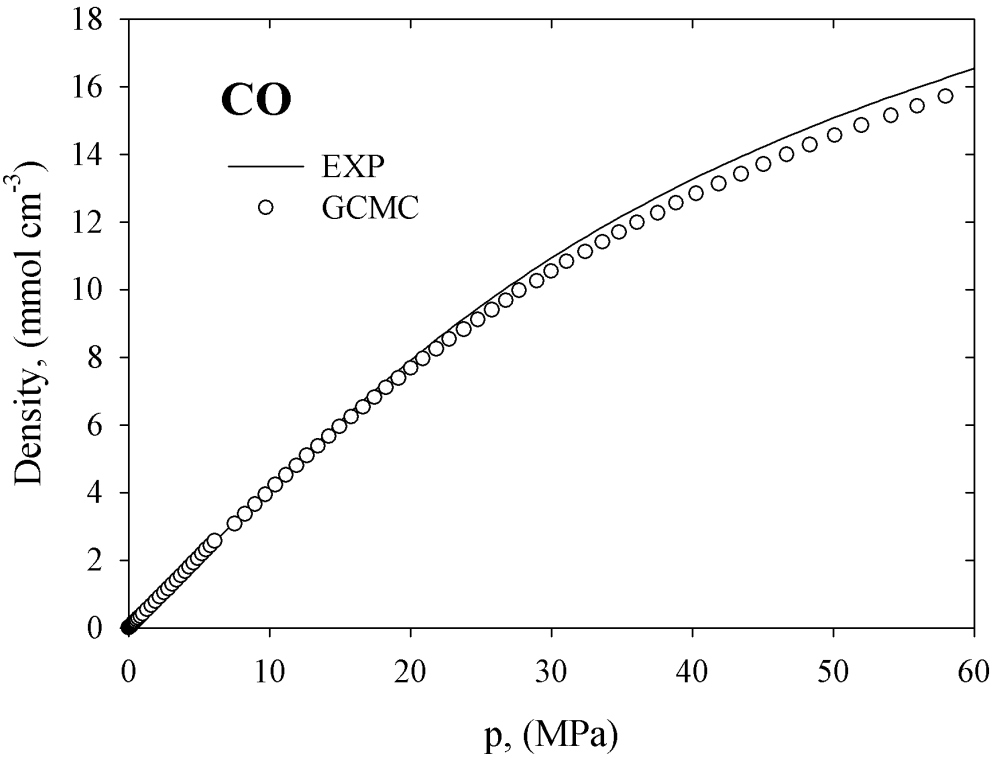

Figure 1S. Comparison of the experimental equation of states for CO fluid at 298 K (solid lines) [1] with the ones computed from Monte Carlo simulations in the grand canonical ensemble (open circles). For CO molecules, we used the 3-site atomistic model of Vrabec *et al.* [4] with bias insertion and deletion moves in GCMC (BGCMC).

References

(1) http://www.nist.gov/index.html

(2) Belof, J. L.; Stern, A. C.; Space, B. An Accurate and Transferable Intermolecular Diatomic Hydrogen Potential For Condensed Phase Simulation *J. Chem. Theory Comput.* **2008**, *4*, 1332-1337.

(3) Ceperley, D. M. Path Integrals in The Theory of Condensed Helium *Rev. Mod. Phys.* **1995**, 67, 279-355.

(4) Vrabec, J.; Stoll, J.; Hasse, H. A Set of Molecular Models For Symmetric Quadrupolar Fluids *J. Phys. Chem. B* **2001**, *105*, 12126-12133.