Electronic Supplementary Material (ESI) for Faraday Discussions.

Accelerating electrostatic pair methods on graphical processing units to study molecules in supercritical carbon dioxide

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Electronic Supplementary Information

Pure carbon dioxide at 323.2 K

For pure carbon dioxide we investigated the temperature 323.2 K alongside 308.2 K, which we reported in the main text. We observe almost identical results for PPPM and the Wolf method, for both the PVT relationship and diffusion coefficients.

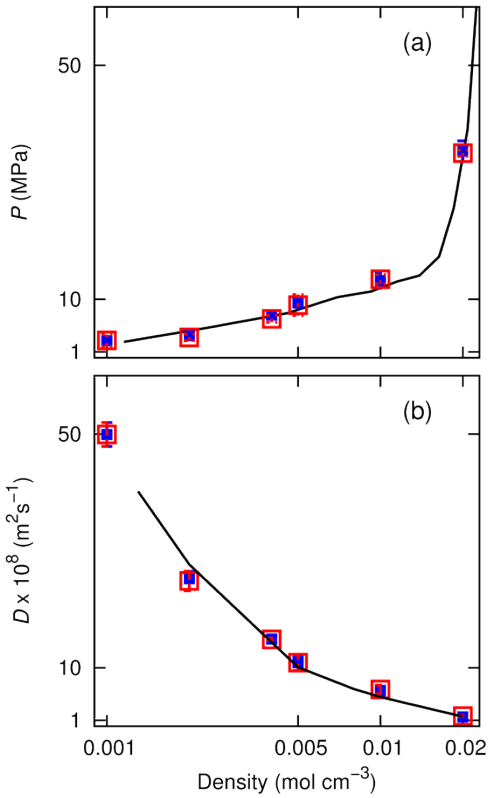

Fig. S1 a) Diffusion coefficients for pure carbon dioxide obtained for PPPM (empty red squares) and Wolf (filled blue squares), compared with experimental (black line) at 323.2 K. b) PVT relationship of pure carbon dioxide simulated using PPPM (empty red squares) or the Wolf method (filled blue squares) compared with experimental (black line) at 323.2 K.