Supplementary Material for “Janus van der Waals equations for real molecules with two-sided phase transitions”

Jihwan Kim , Do-Hyun Kim , and Jeong-Hyuck Park

1 SUPPLEMENTARY FIGURES FOR $\mathrm{N}=4$ CASE

1.1 argon (Ar)

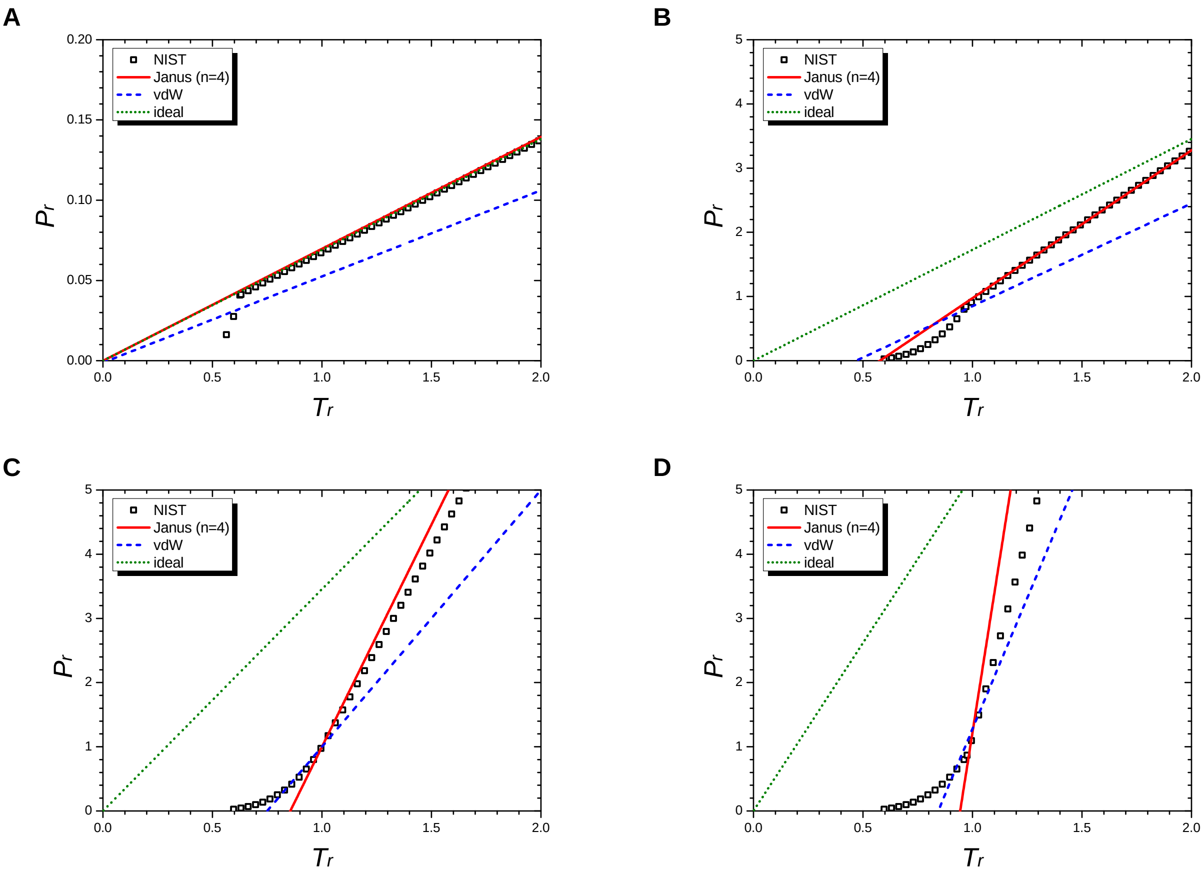

Figure S1. Isochoric curves of argon (Ar) at $1/v_r = 0.02$ (**A**), $1/v_r = 0.5$ (**B**), $1/v_r = 1.0$ (**C**), and $1/v_r = 1.5$ (**D**). Boxes are from the NIST data. The red solid line is drawn from the $n = 4$ Janus van der Waals equation, the blue dashed line from the original van der Waals equation, and the green dotted line from the classical ideal gas law.

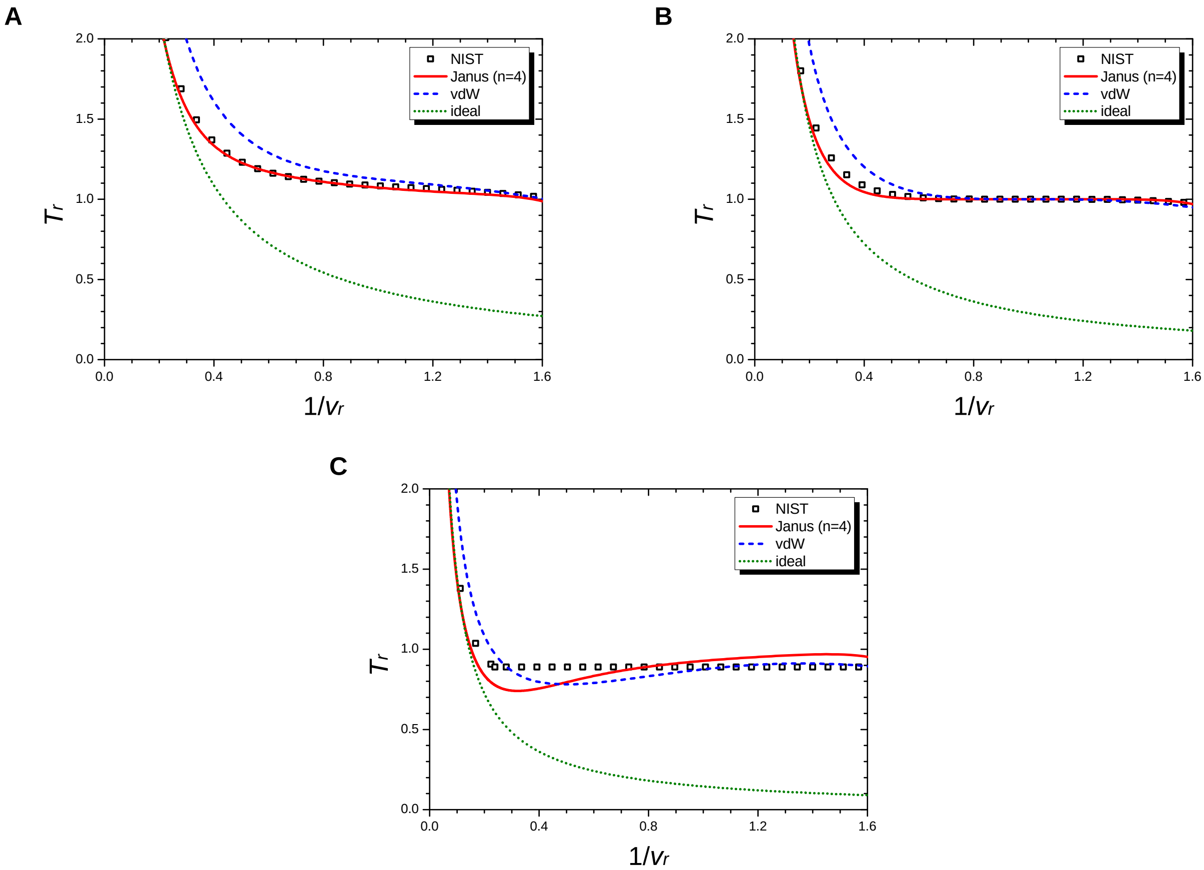

Figure S2. Isobaric curves of argon (Ar) at $P_r = 1.5$ (**A**), $P_r = 1.0$ (**B**), and $P_r = 0.5$ (**C**). Boxes are from the NIST data. The red solid line is drawn from the $n = 4$ Janus van der Waals equation, the blue dashed line from the original van der Waals equation, and the green dotted line from the classical ideal gas law.

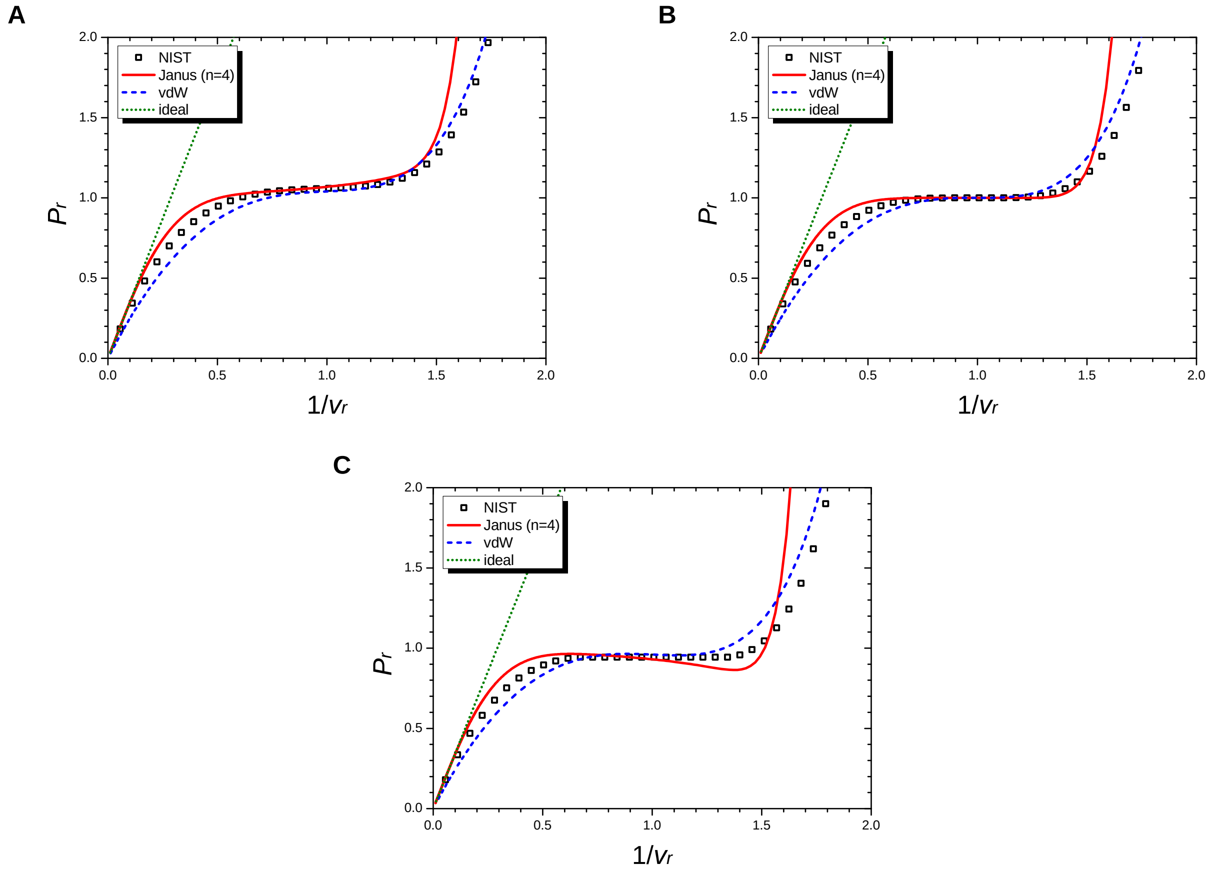

Figure S3. Isothermal curves of argon (Ar) at $T_r = 1.01$ (**A**), $T_r = 1.00$ (**B**), and $T_r = 0.99$ (**C**). Boxes are from the NIST data. The red solid line is drawn from the $n = 4$ Janus van der Waals equation, the blue dashed line from the original van der Waals equation, and the green dotted line from the classical ideal gas law.

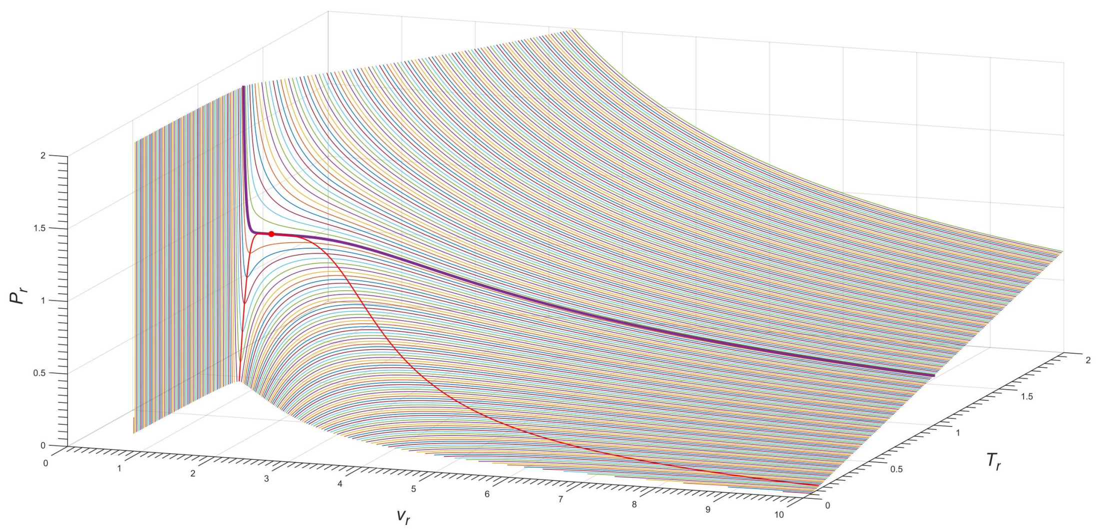

Figure S4. Three-dimensional $P_r - v_r - T_r$ phase diagram of the exact $n = 4$ Janus van der Waals equation, as for argon (Ar). The bold purple line corresponds to the isotherm of $T_r = 1.00$ as depicted in **Figure S3 B**; the red line is the Janus van der Waals spinodal curve with $a = 0.99$; and the red dot is the critical point.

1.2 methane (CH_4)

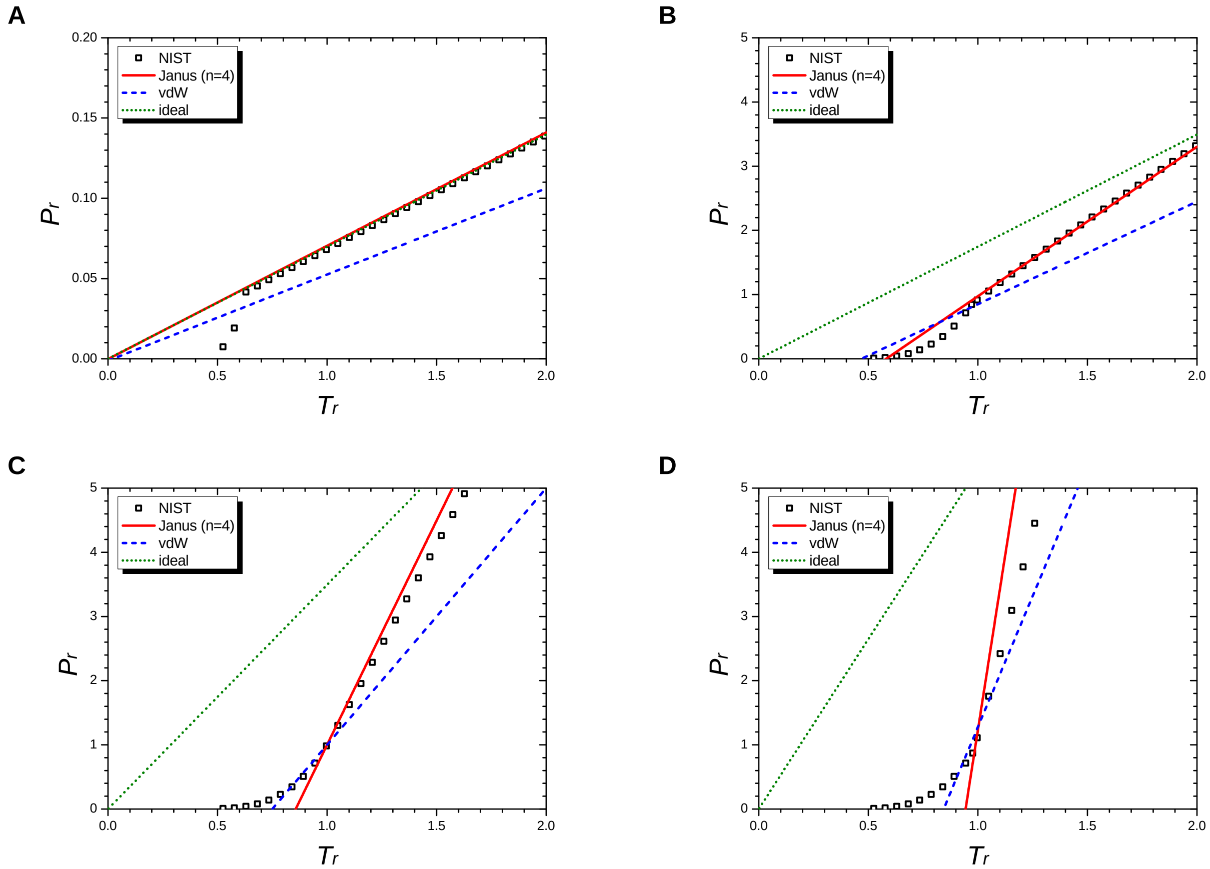

Figure S5. Isochoric curves of methane (CH_4) at $1/v_r = 0.02$ (**A**), $1/v_r = 0.5$ (**B**), $1/v_r = 1.0$ (**C**), and $1/v_r = 1.5$ (**D**). Boxes are from the NIST data. The red solid line is drawn from the $n = 4$ Janus van der Waals equation, the blue dashed line from the original van der Waals equation, and the green dotted line from the classical ideal gas law.

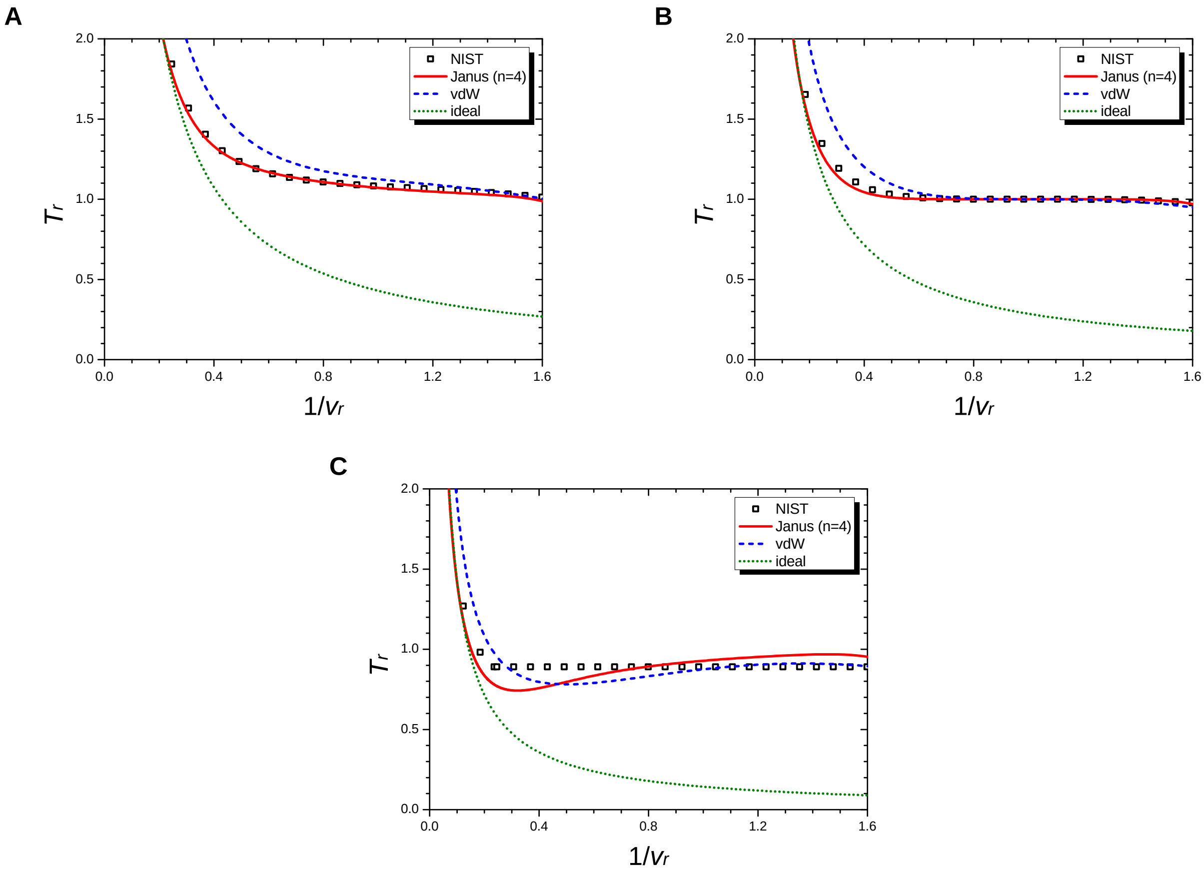

Figure S6. Isobaric curves of methane (CH_4) at $P_r = 1.5$ (**A**), $P_r = 1.0$ (**B**), and $P_r = 0.5$ (**C**). Boxes are from the NIST data. The red solid line is drawn from the $n = 4$ Janus van der Waals equation, the blue dashed line from the original van der Waals equation, and the green dotted line from the classical ideal gas law.

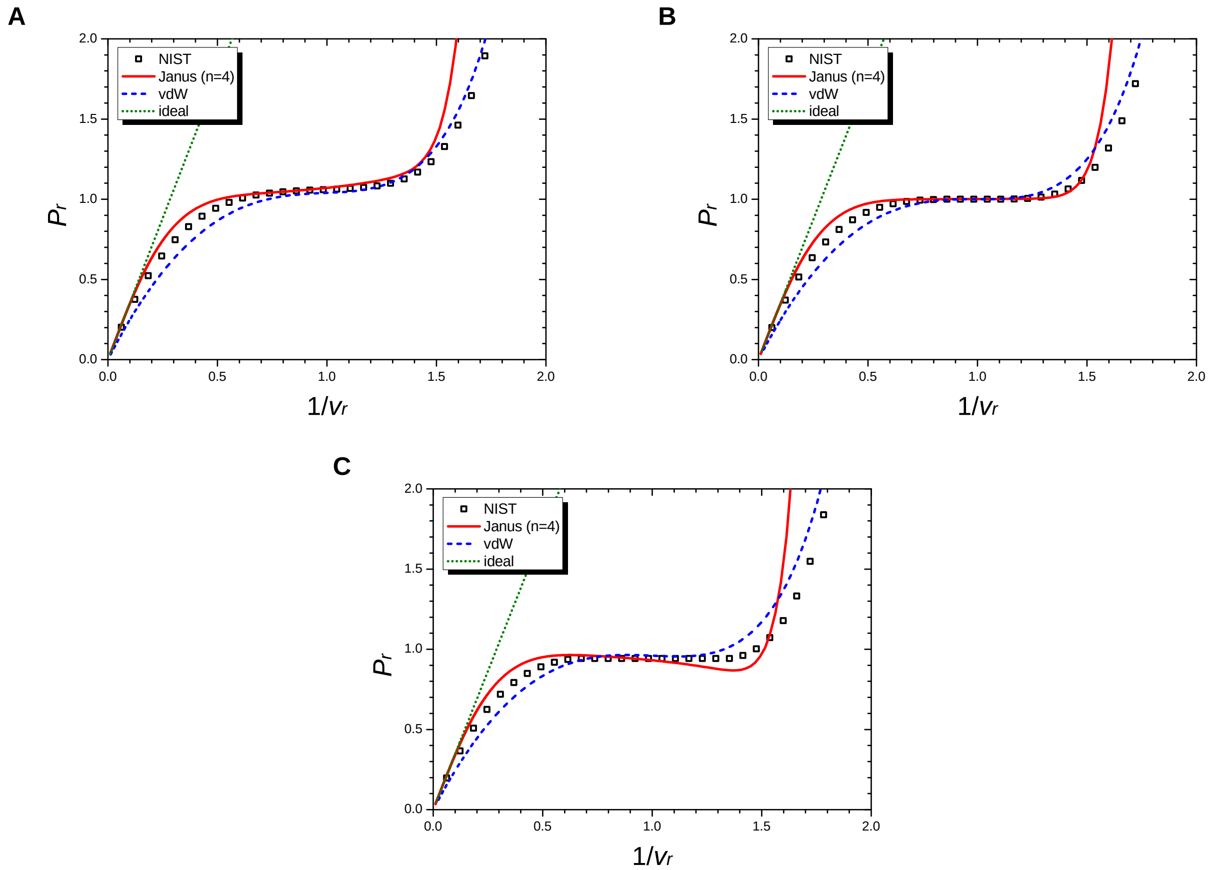

Figure S7. Isothermal curves of methane (CH_4) at $T_r = 1.01$ (**A**), $T_r = 1.00$ (**B**), and $T_r = 0.99$ (**C**). Boxes are from the NIST data. The red solid line is drawn from the $n = 4$ Janus van der Waals equation, the blue dashed line from the original van der Waals equation, and the green dotted line from the classical ideal gas law.

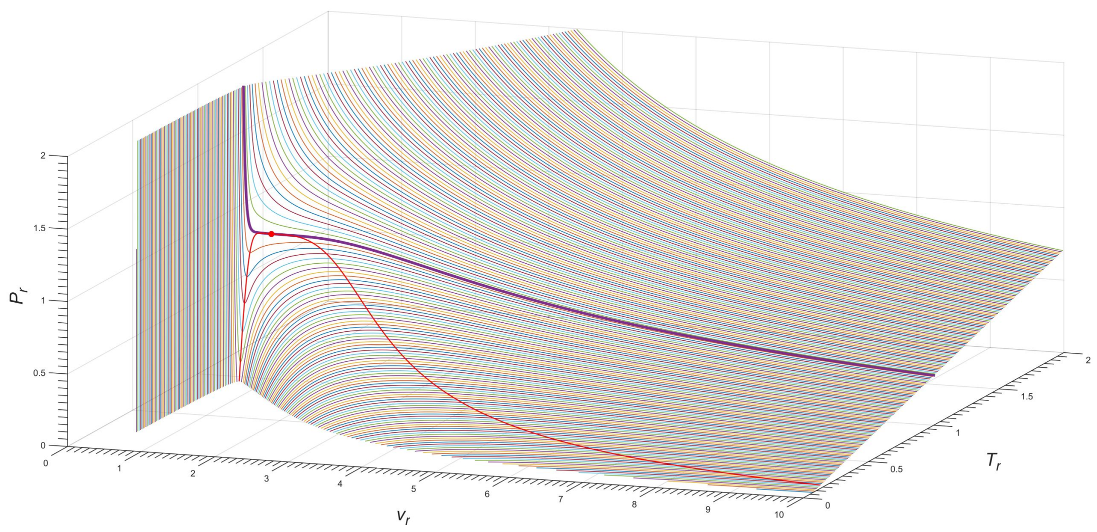

Figure S8. Three-dimensional $P_r - v_r - T_r$ phase diagram of the exact $n = 4$ Janus van der Waals equation, as for methane ($\mathrm{CH_4}$). The bold purple line corresponds to the isotherm of $T_r = 1.00$ as depicted in **Figure S7 B**; the red line is the Janus van der Waals spinodal curve with $a = 0.99$; and the red dot is the critical point.

1.3 ethylene (C_2H_4)

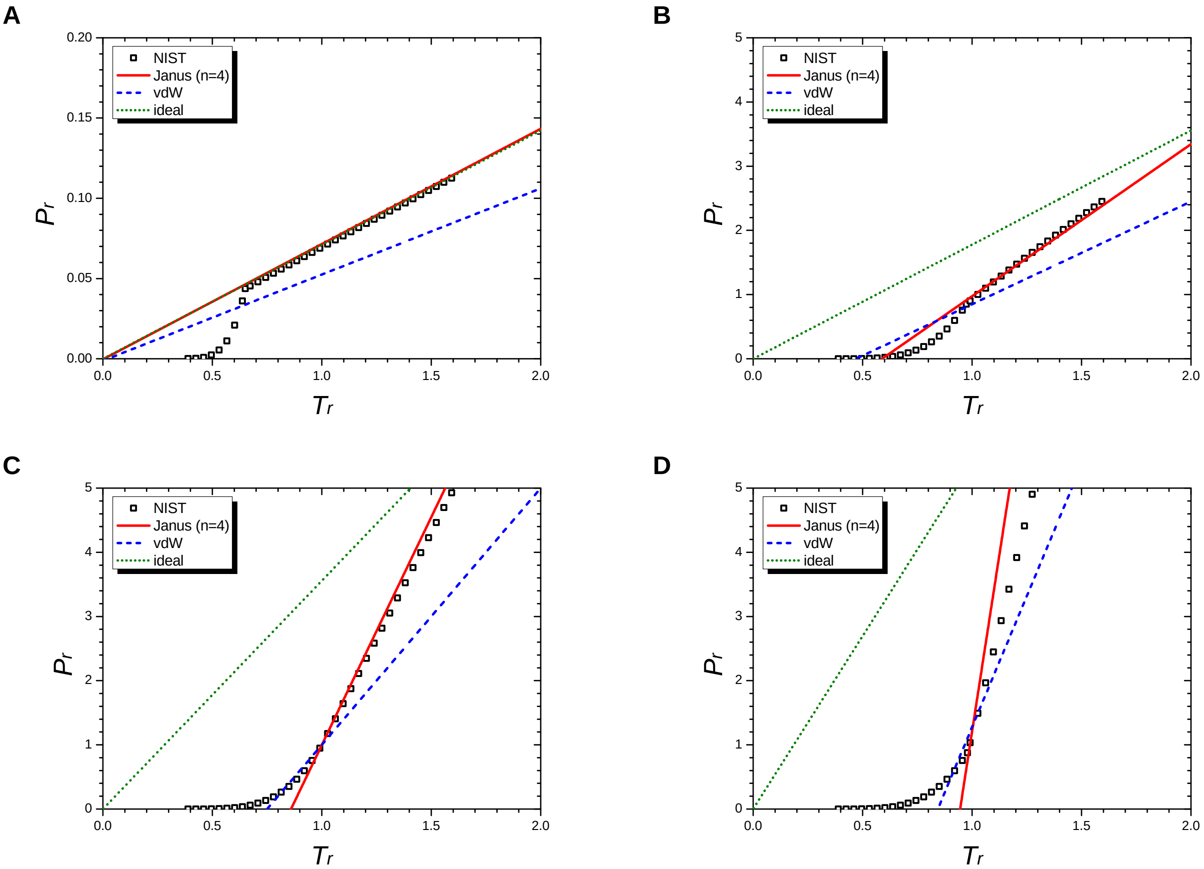

Figure S9. Isochoric curves of ethylene (C_2H_4) at $1/v_r = 0.02$ (**A**), $1/v_r = 0.5$ (**B**), $1/v_r = 1.0$ (**C**), and $1/v_r = 1.5$ (**D**). Boxes are from the NIST data. The red solid line is drawn from the $n = 4$ Janus van der Waals equation, the blue dashed line from the original van der Waals equation, and the green dotted line from the classical ideal gas law.

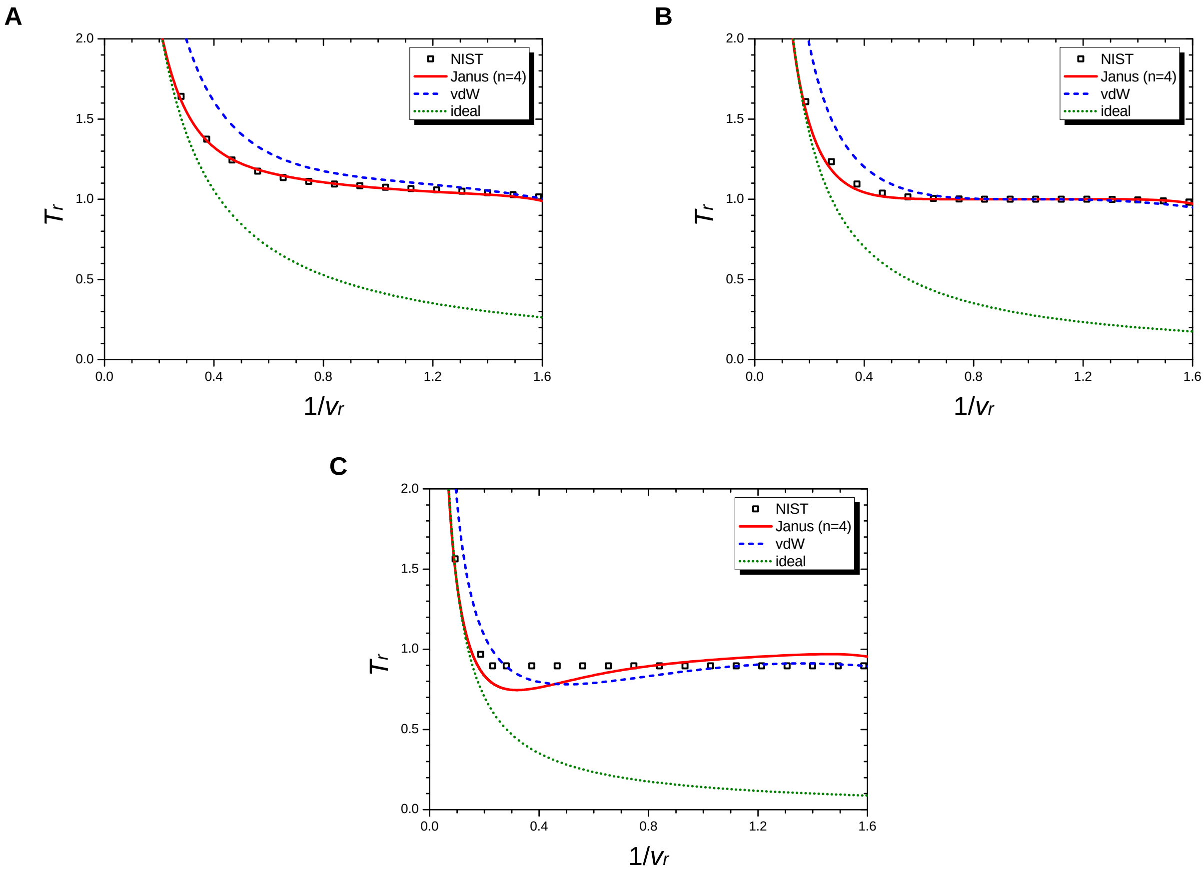

Figure S10. Isobaric curves of ethylene (C_2H_4) at $P_r = 1.5$ (**A**), $P_r = 1.0$ (**B**), and $P_r = 0.5$ (**C**). Boxes are from the NIST data. The red solid line is drawn from the $n = 4$ Janus van der Waals equation, the blue dashed line from the original van der Waals equation, and the green dotted line from the classical ideal gas law.

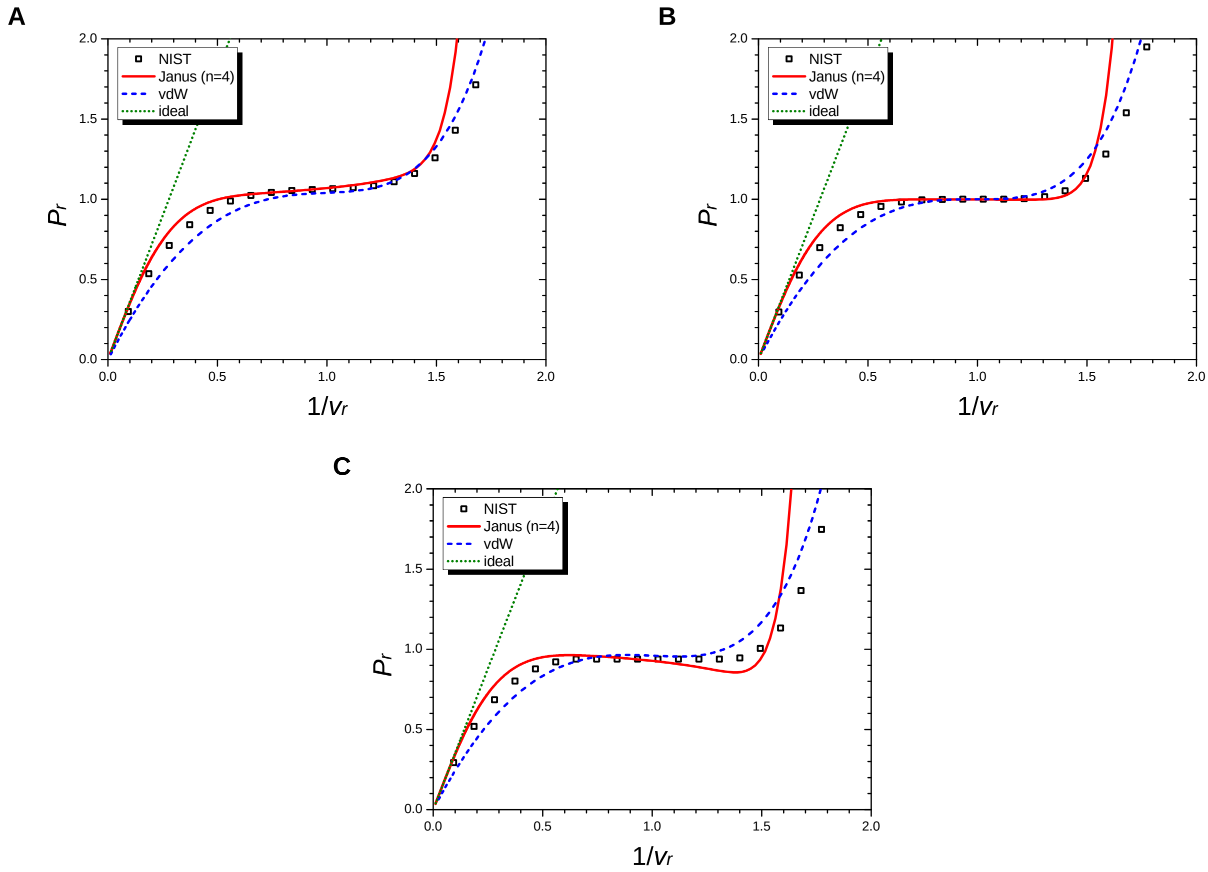

Figure S11. Isothermal curves of ethylene (C_2H_4) at $T_r = 1.01$ (**A**), $T_r = 1.00$ (**B**), and $T_r = 0.99$ (**C**). Boxes are from the NIST data. The red solid line is drawn from the $n = 4$ Janus van der Waals equation, the blue dashed line from the original van der Waals equation, and the green dotted line from the classical ideal gas law.

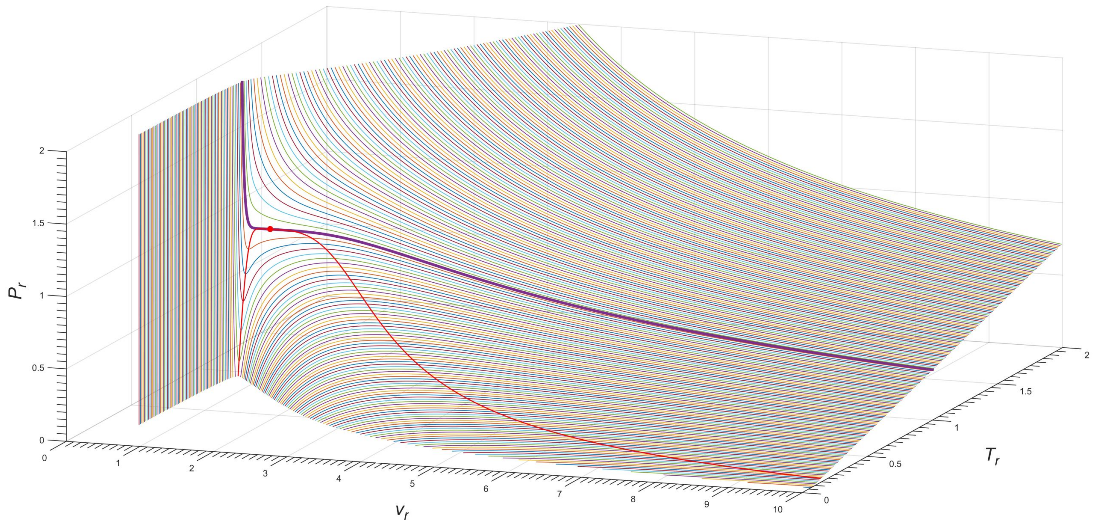

Figure S12. Three-dimensional $P_r - v_r - T_r$ phase diagram of the exact $n = 4$ Janus van der Waals equation, as for ethylene ($\mathrm{C_2H_4}$). The bold purple line corresponds to the isotherm of $T_r = 1.00$ as depicted in **Figure S11 B**; the red line is the Janus van der Waals spinodal curve with $a = 0.99$; and the red dot is the critical point.

1.4 ethane (C_2H_6)

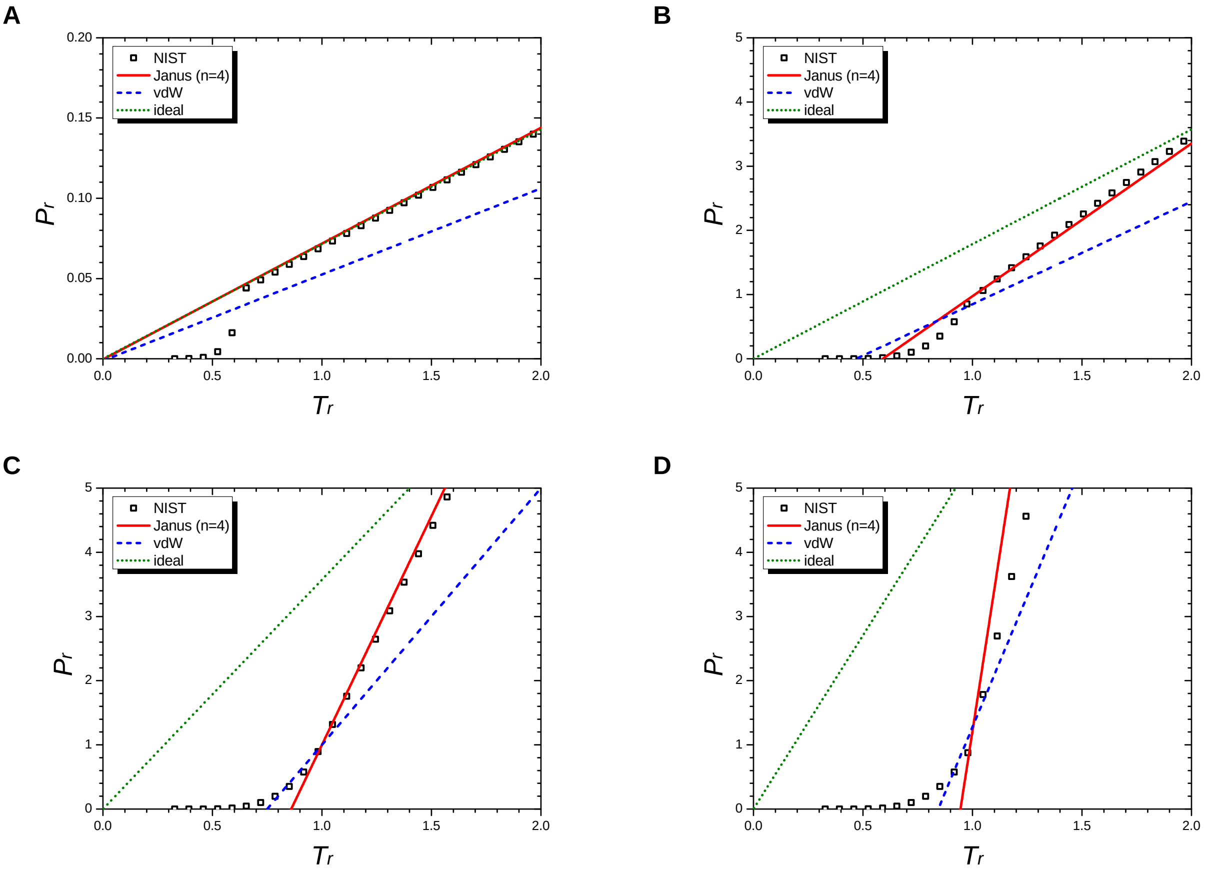

Figure S13. Isochoric curves of ethane (C_2H_6) at $1/v_r = 0.02$ (**A**), $1/v_r = 0.5$ (**B**), $1/v_r = 1.0$ (**C**), and $1/v_r = 1.5$ (**D**). Boxes are from the NIST data. The red solid line is drawn from the $n = 4$ Janus van der Waals equation, the blue dashed line from the original van der Waals equation, and the green dotted line from the classical ideal gas law.

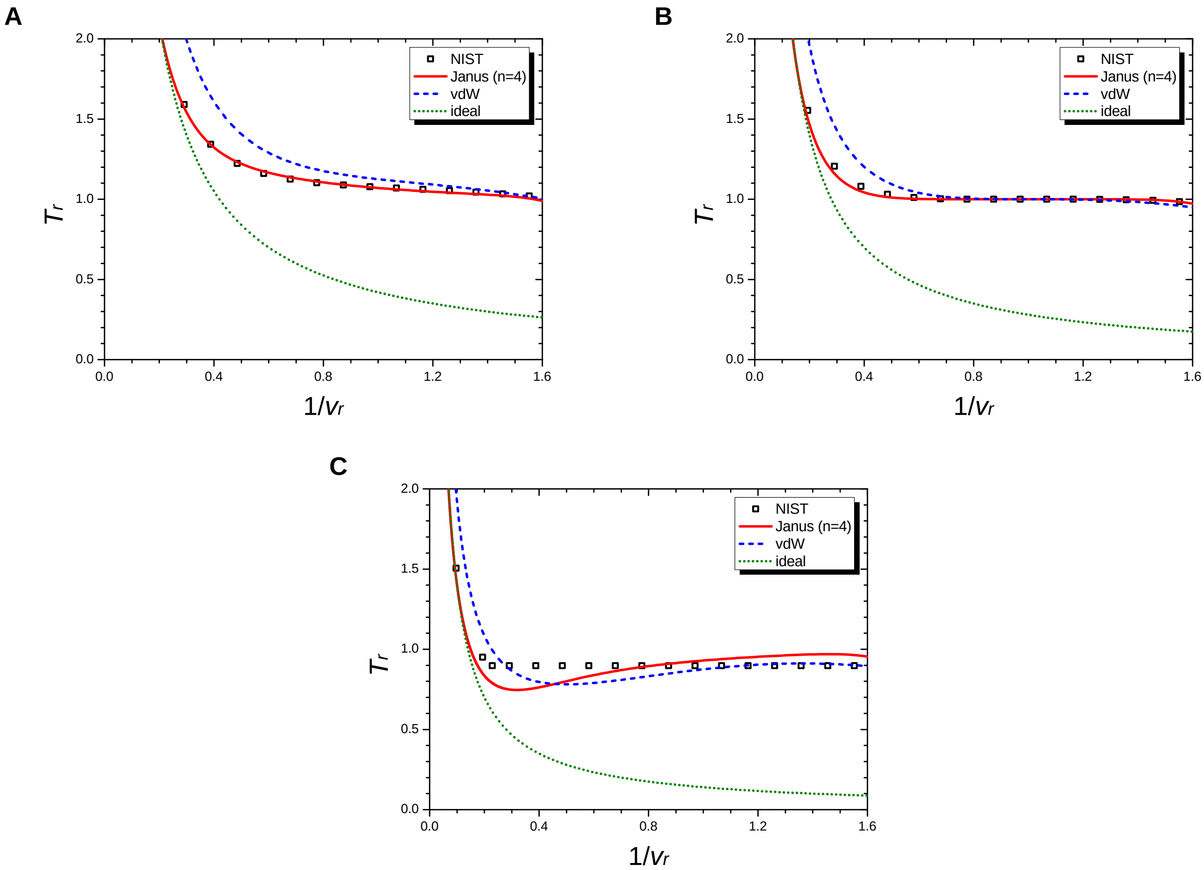

Figure S14. Isobaric curves of ethane (C_2H_6) at $P_r = 1.5$ (**A**), $P_r = 1.0$ (**B**), and $P_r = 0.5$ (**C**). Boxes are from the NIST data. The red solid line is drawn from the $n = 4$ Janus van der Waals equation, the blue dashed line from the original van der Waals equation, and the green dotted line from the classical ideal gas law.

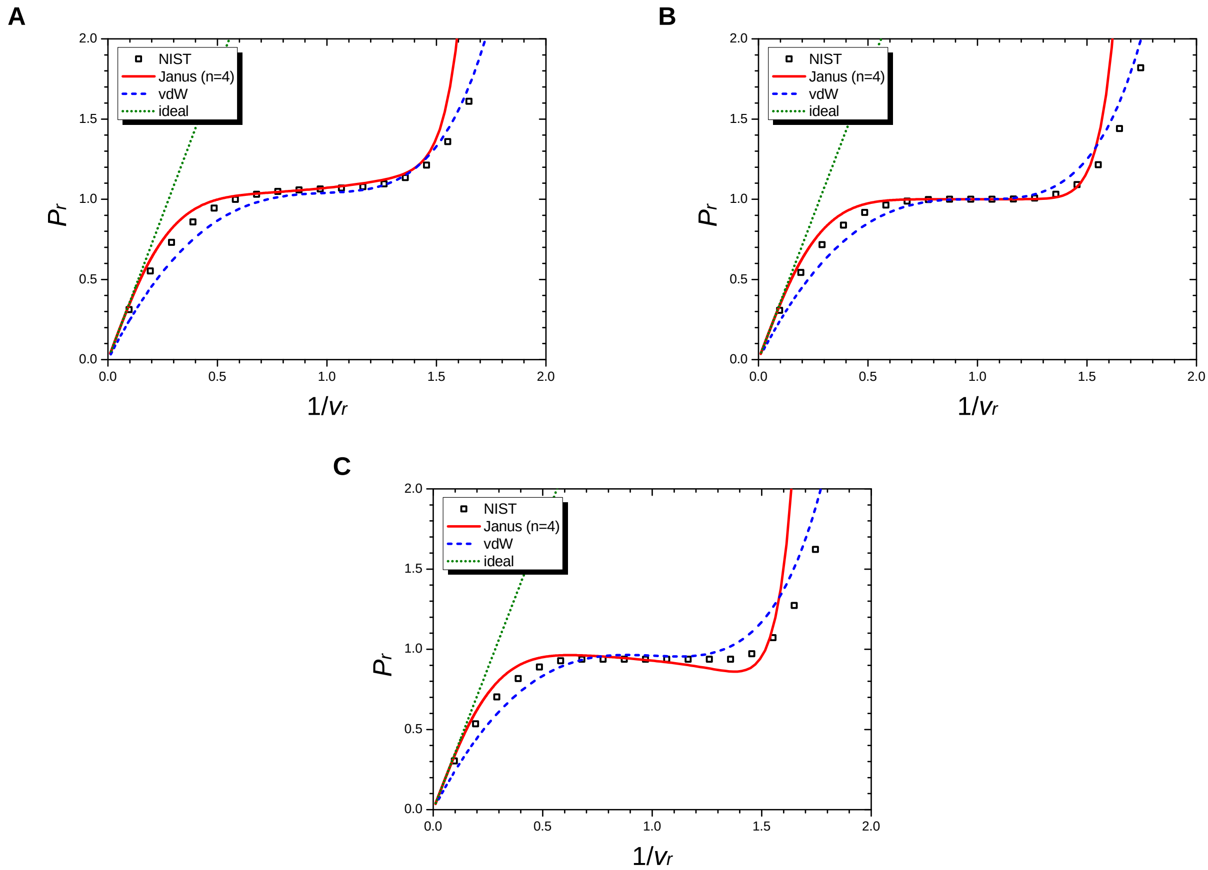

Figure S15. Isothermal curves of ethane (C_2H_6) at $T_r = 1.01$ (**A**), $T_r = 1.00$ (**B**), and $T_r = 0.99$ (**C**). Boxes are from the NIST data. The red solid line is drawn from the $n = 4$ Janus van der Waals equation, the blue dashed line from the original van der Waals equation, and the green dotted line from the classical ideal gas law.

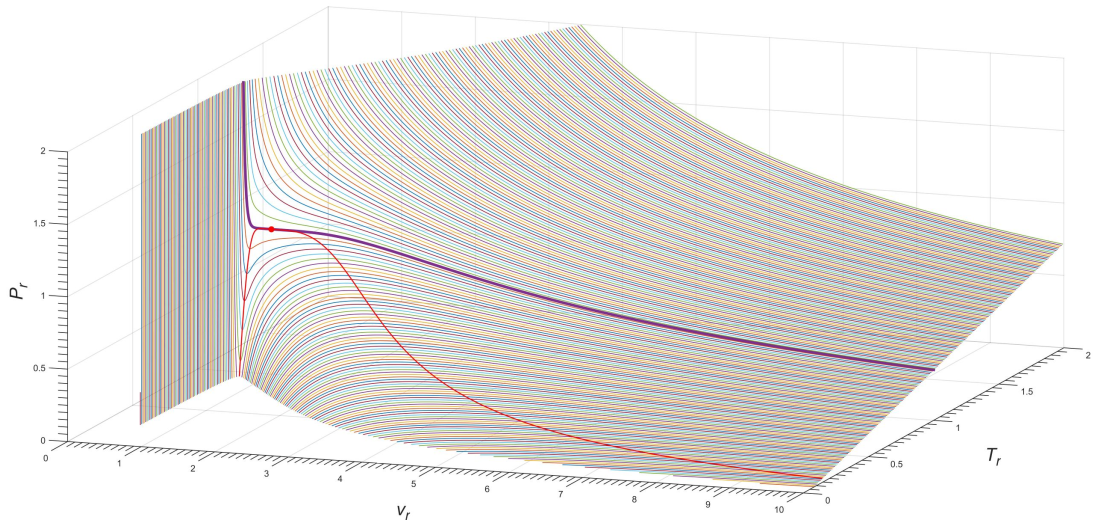

Figure S16. Three-dimensional $P_r - v_r - T_r$ phase diagram of the exact $n = 4$ Janus van der Waals equation, as for ethane (C_2H_6). The bold purple line corresponds to the isotherm of $T_r = 1.00$ as depicted in **Figure S15 B**; the red line is the Janus van der Waals spinodal curve with $a = 0.99$; and the red dot is the critical point.

1.5 propylene (C_3H_6)

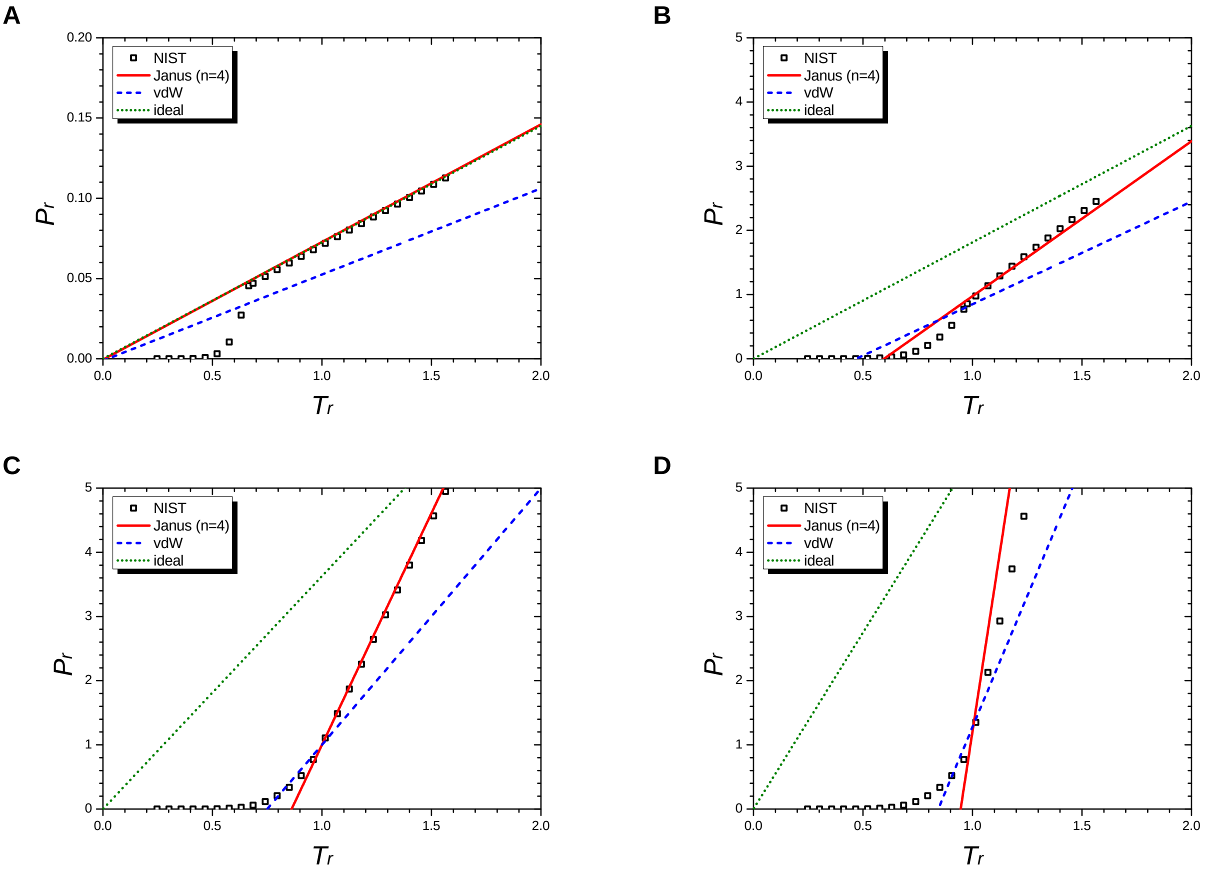

Figure S17. Isochoric curves of propylene (C_3H_6) at $1/v_r = 0.02$ (**A**), $1/v_r = 0.5$ (**B**), $1/v_r = 1.0$ (**C**), and $1/v_r = 1.5$ (**D**). Boxes are from the NIST data. The red solid line is drawn from the $n = 4$ Janus van der Waals equation, the blue dashed line from the original van der Waals equation, and the green dotted line from the classical ideal gas law.

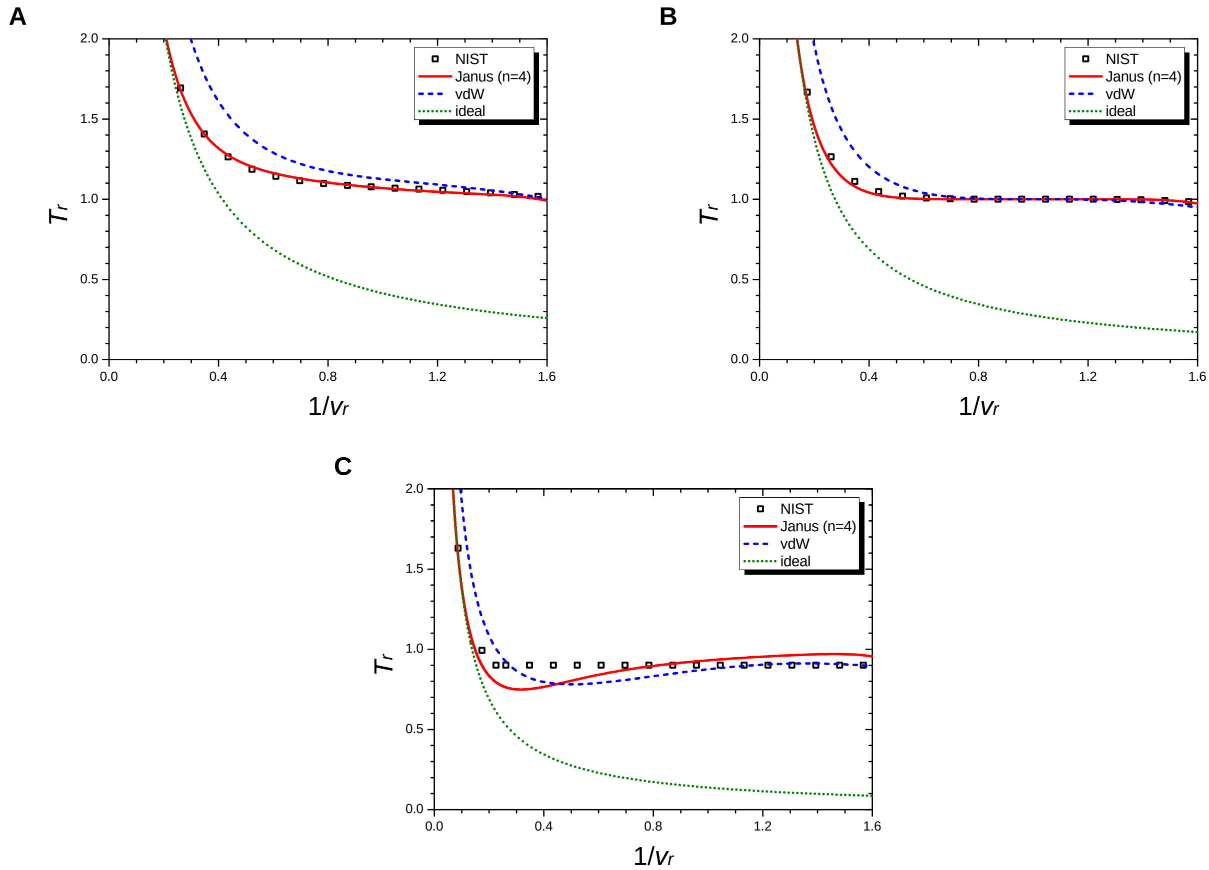

Figure S18. Isobaric curves of propylene (C_3H_6) at $P_r = 1.5$ (**A**), $P_r = 1.0$ (**B**), and $P_r = 0.5$ (**C**). Boxes are from the NIST data. The red solid line is drawn from the $n = 4$ Janus van der Waals equation, the blue dashed line from the original van der Waals equation, and the green dotted line from the classical ideal gas law.

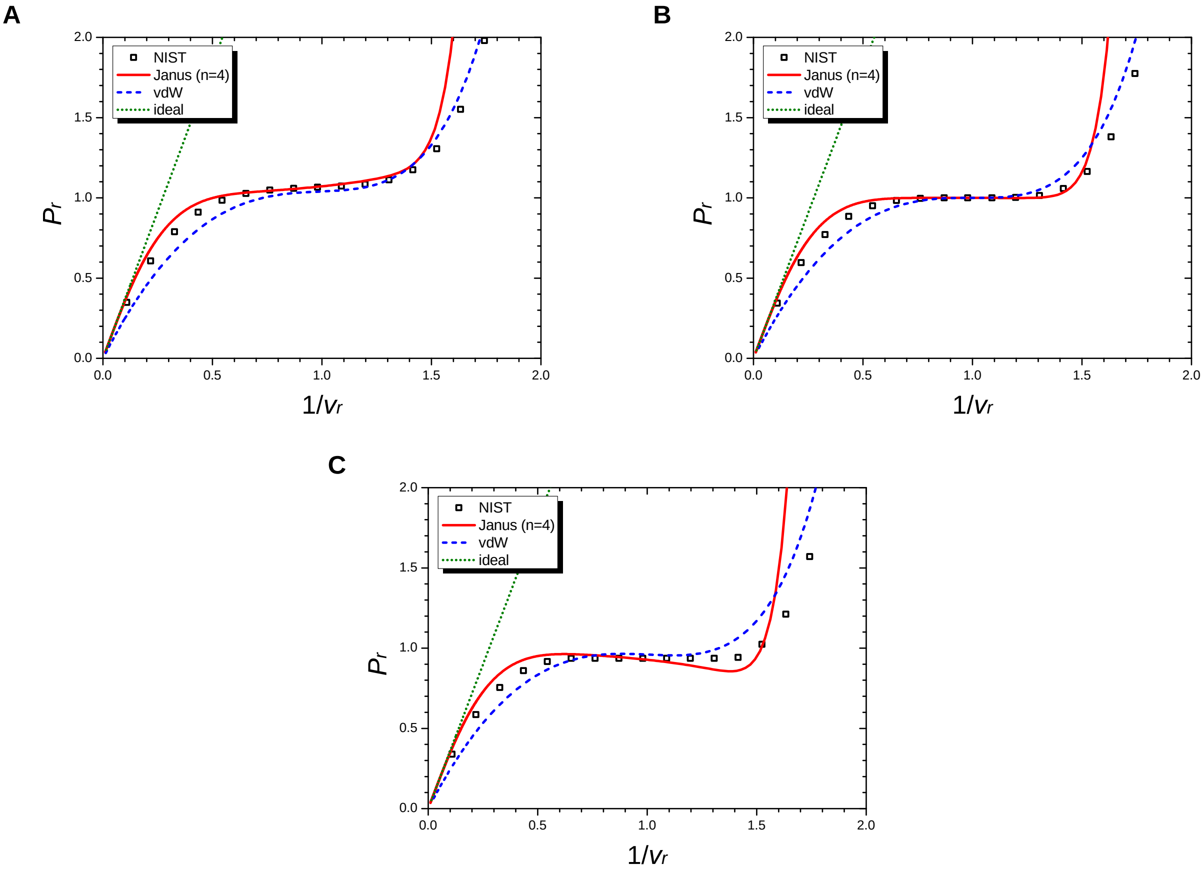

Figure S19. Isothermal curves of propylene (C_3H_6) at $T_r = 1.01$ (**A**), $T_r = 1.00$ (**B**), and $T_r = 0.99$ (**C**). Boxes are from the NIST data. The red solid line is drawn from the $n = 4$ Janus van der Waals equation, the blue dashed line from the original van der Waals equation, and the green dotted line from the classical ideal gas law.

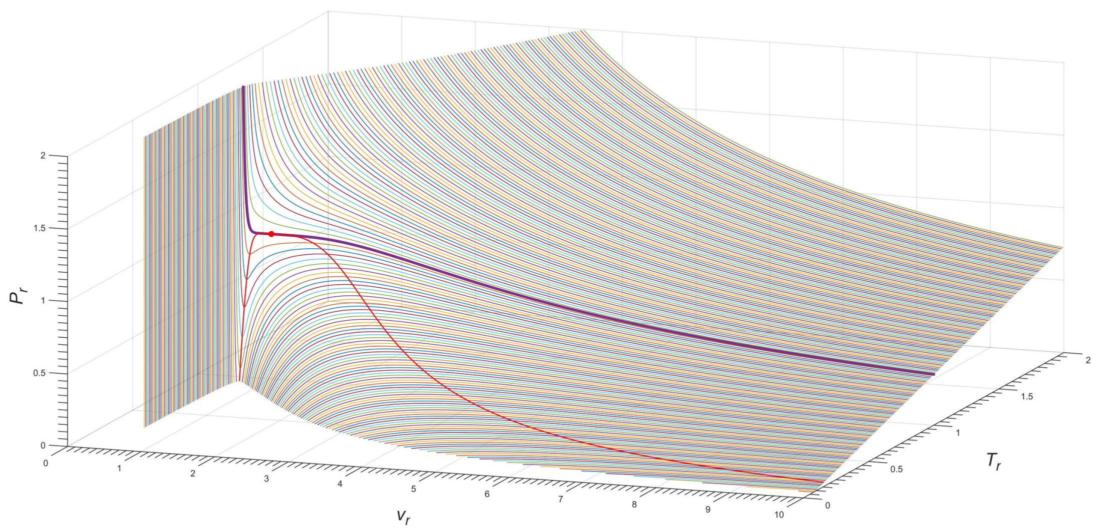

Figure S20. Three-dimensional $P_r - v_r - T_r$ phase diagram of the exact $n = 4$ Janus van der Waals equation, as for propylene ($\mathrm{C_3H_6}$). The bold purple line corresponds to the isotherm of $T_r = 1.00$ as depicted in **Figure S19 B**; the red line is the Janus van der Waals spinodal curve with $a = 0.99$; and the red dot is the critical point.

1.6 propane (C_3H_8)

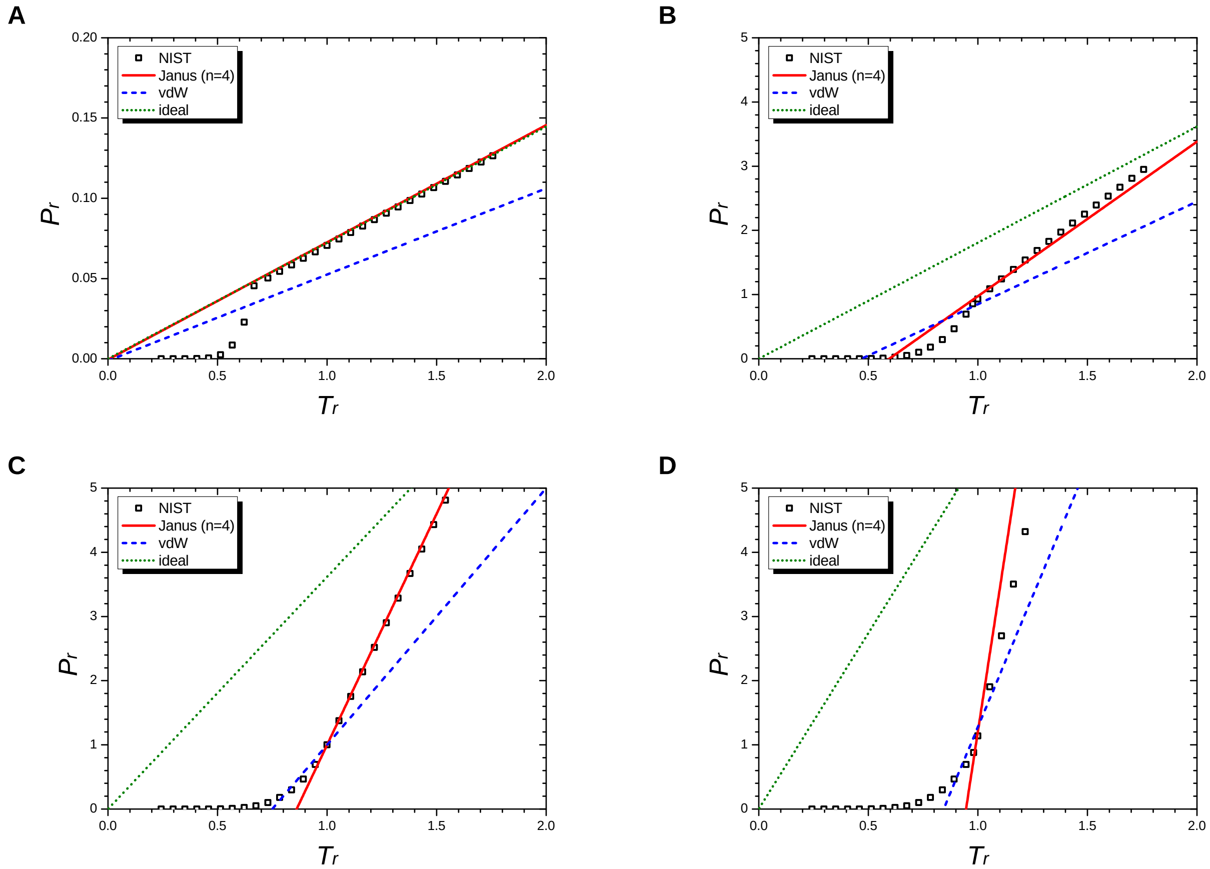

Figure S21. Isochoric curves of propane (C_3H_8) at $1/v_r = 0.02$ (**A**), $1/v_r = 0.5$ (**B**), $1/v_r = 1.0$ (**C**), and $1/v_r = 1.5$ (**D**). Boxes are from the NIST data. The red solid line is drawn from the $n = 4$ Janus van der Waals equation, the blue dashed line from the original van der Waals equation, and the green dotted line from the classical ideal gas law.

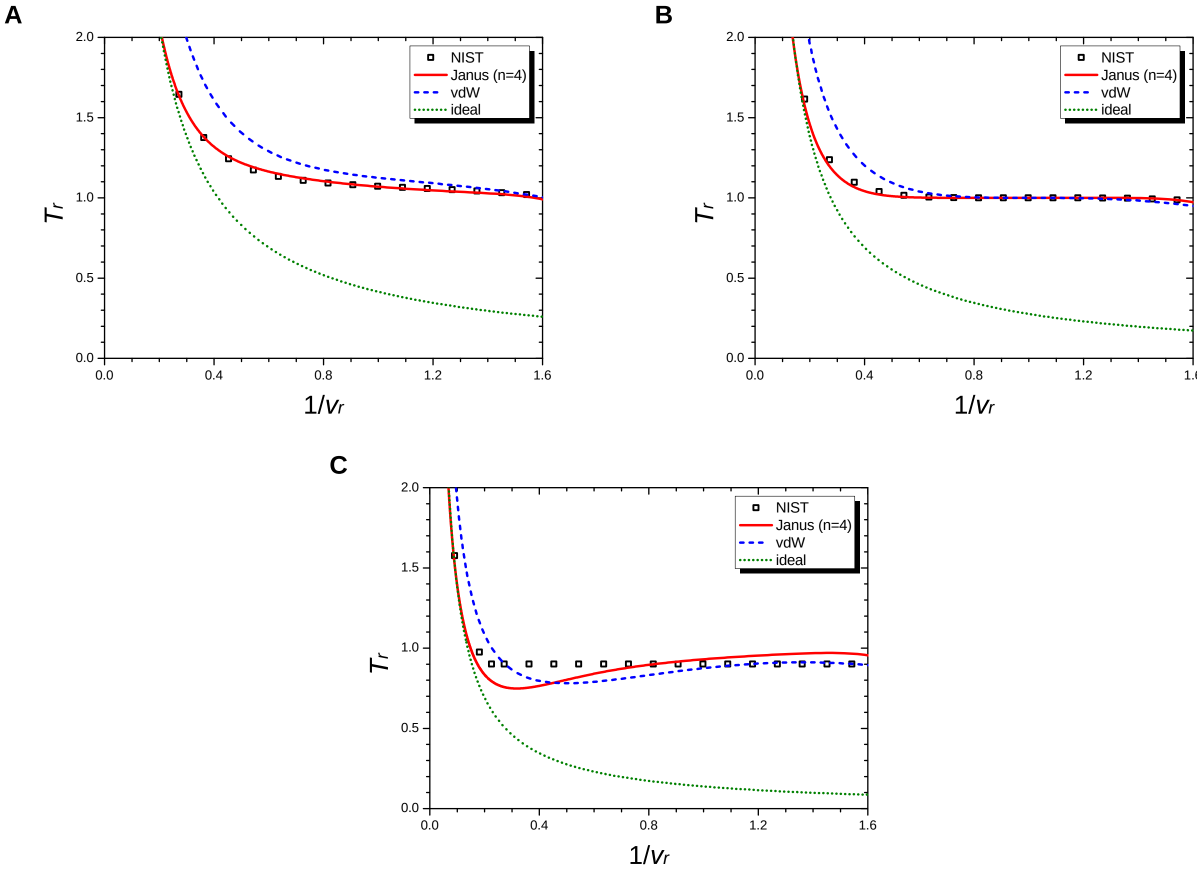

Figure S22. Isobaric curves of propane (C_3H_8) at $P_r = 1.5$ (**A**), $P_r = 1.0$ (**B**), and $P_r = 0.5$ (**C**). Boxes are from the NIST data. The red solid line is drawn from the $n = 4$ Janus van der Waals equation, the blue dashed line from the original van der Waals equation, and the green dotted line from the classical ideal gas law.

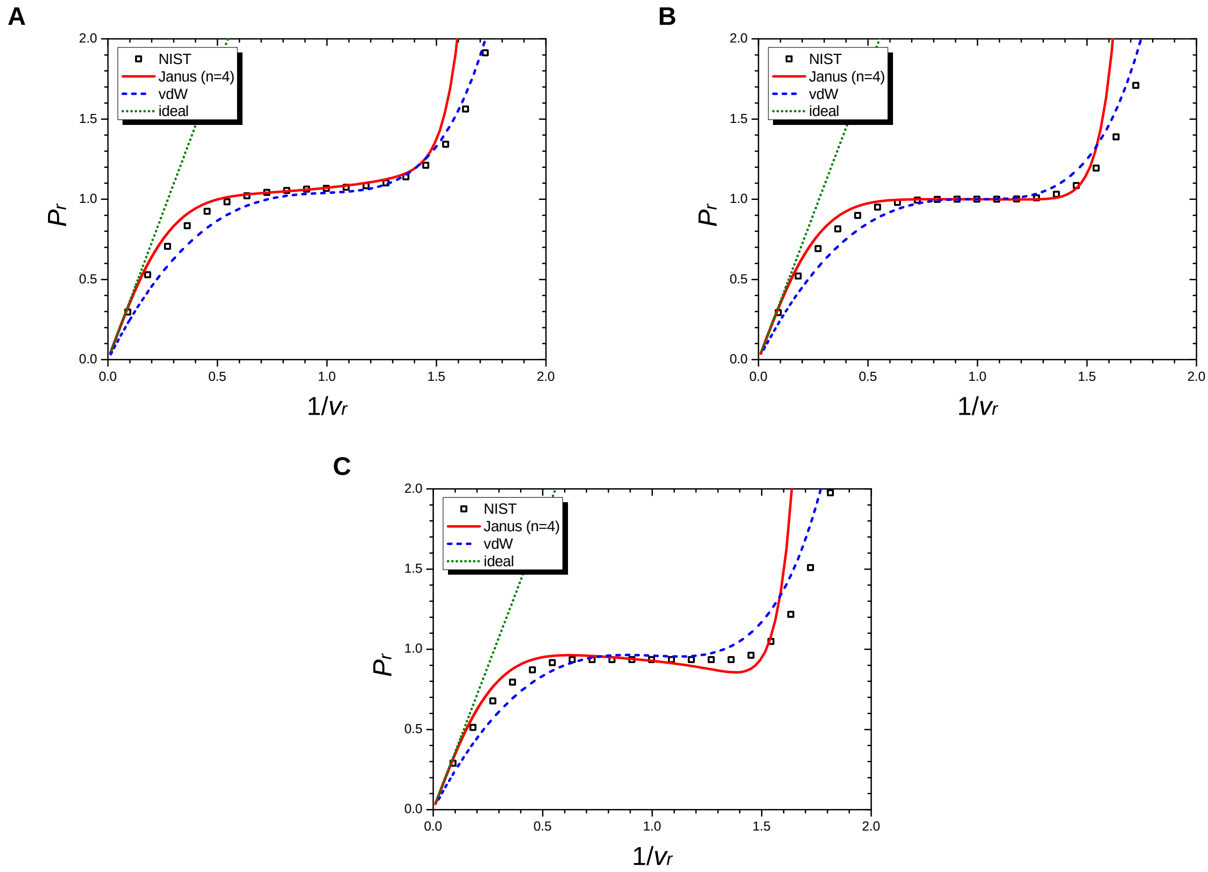

Figure S23. Isothermal curves of propane (C_3H_8) at $T_r = 1.01$ (**A**), $T_r = 1.00$ (**B**), and $T_r = 0.99$ (**C**). Boxes are from the NIST data. The red solid line is drawn from the $n = 4$ Janus van der Waals equation, the blue dashed line from the original van der Waals equation, and the green dotted line from the classical ideal gas law.

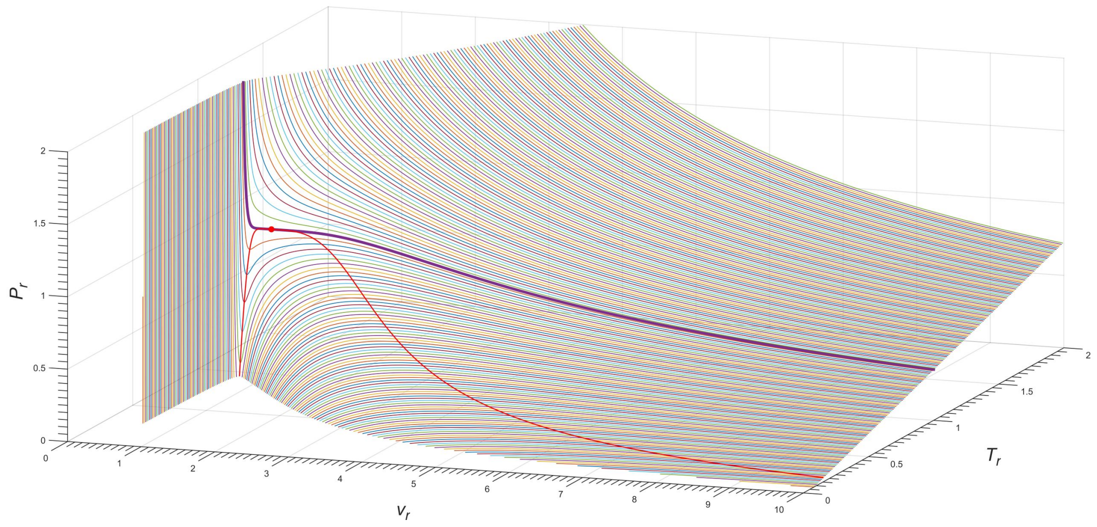

Figure S24. Three-dimensional $P_r - v_r - T_r$ phase diagram of the exact $n = 4$ Janus van der Waals equation, as for propane (C_3H_8). The bold purple line corresponds to the isotherm of $T_r = 1.00$ as depicted in **Figure S23 B**; the red line is the Janus van der Waals spinodal curve with $a = 0.99$; and the red dot is the critical point.

1.7 butane (C_4H_{10})

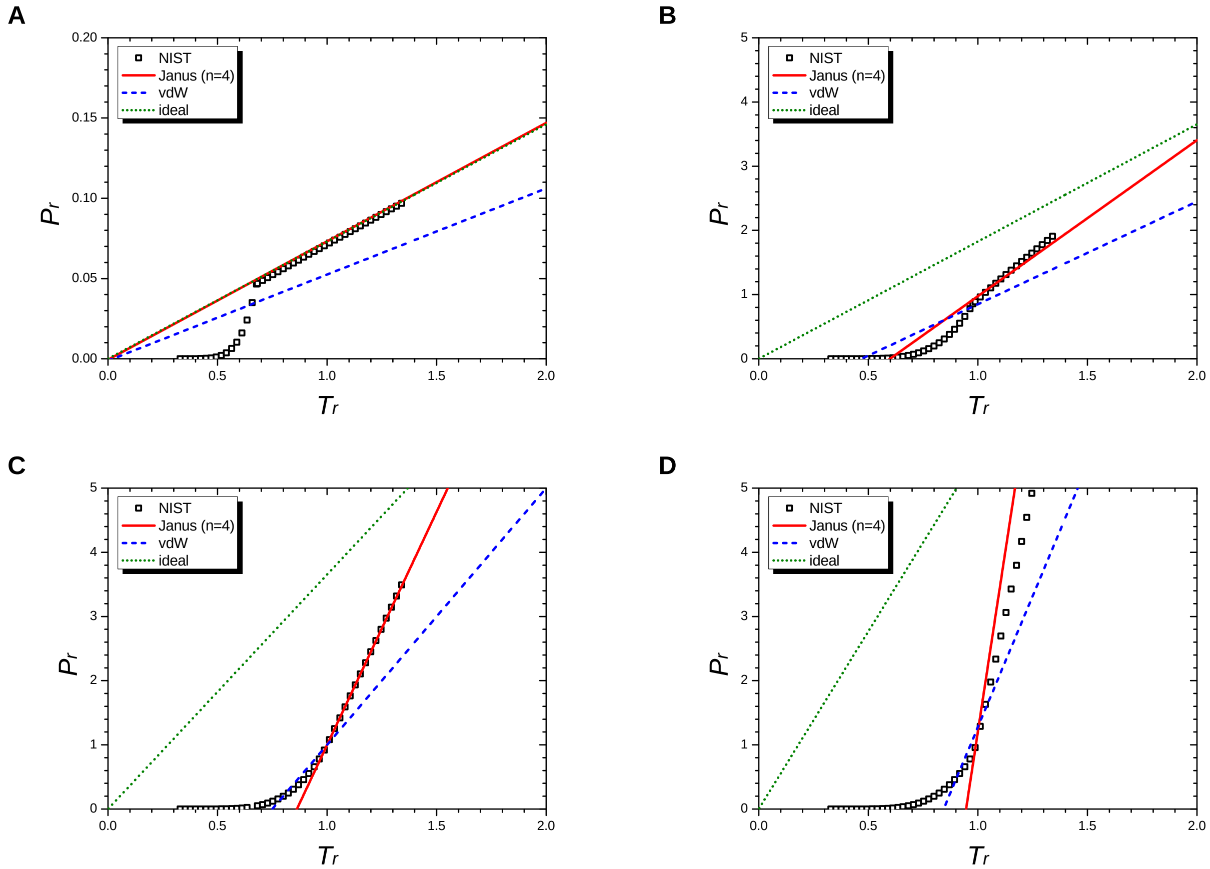

Figure S25. Isochoric curves of butane (C_4H_{10}) at $1/v_r = 0.02$ (**A**), $1/v_r = 0.5$ (**B**), $1/v_r = 1.0$ (**C**), and $1/v_r = 1.5$ (**D**). Boxes are from the NIST data. The red solid line is drawn from the $n = 4$ Janus van der Waals equation, the blue dashed line from the original van der Waals equation, and the green dotted line from the classical ideal gas law.

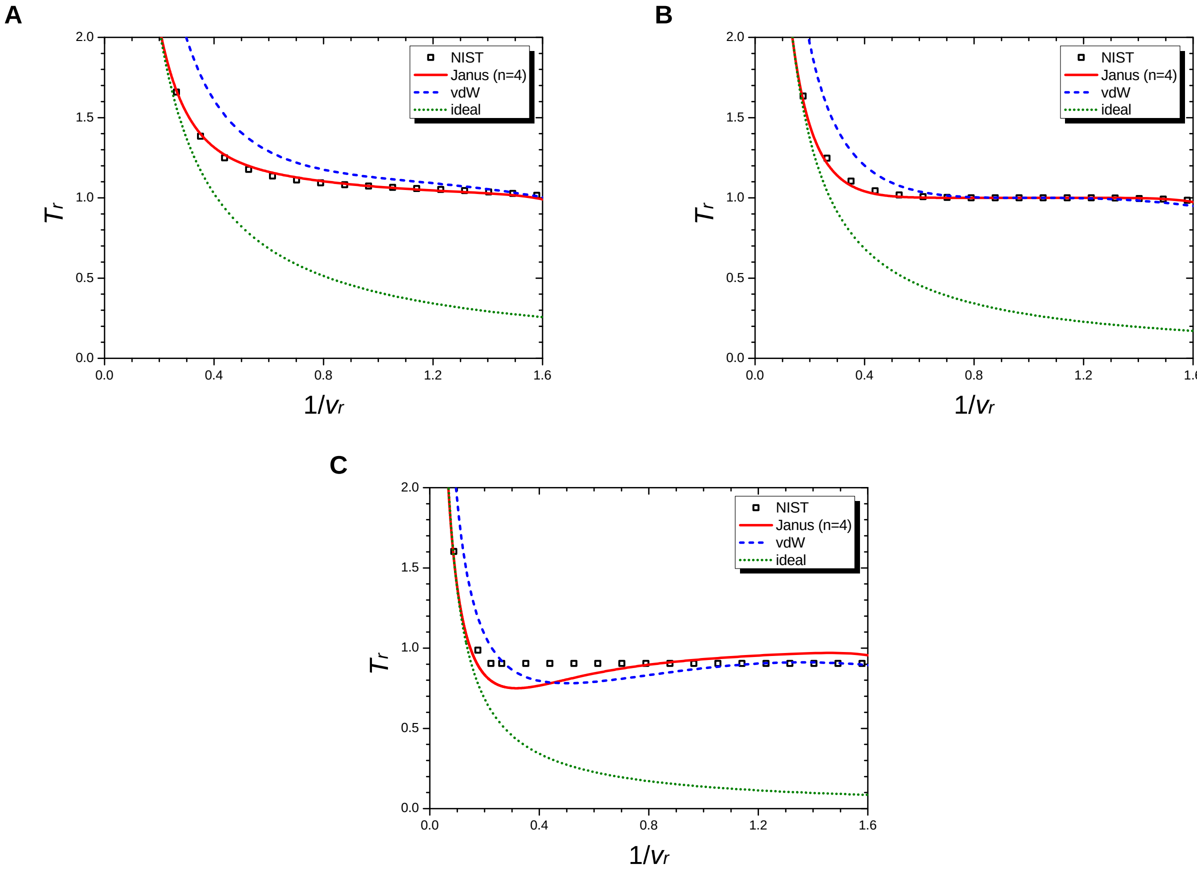

Figure S26. Isobaric curves of butane (C_4H_{10}) at $P_r = 1.5$ (**A**), $P_r = 1.0$ (**B**), and $P_r = 0.5$ (**C**). Boxes are from the NIST data. The red solid line is drawn from the $n = 4$ Janus van der Waals equation, the blue dashed line from the original van der Waals equation, and the green dotted line from the classical ideal gas law.

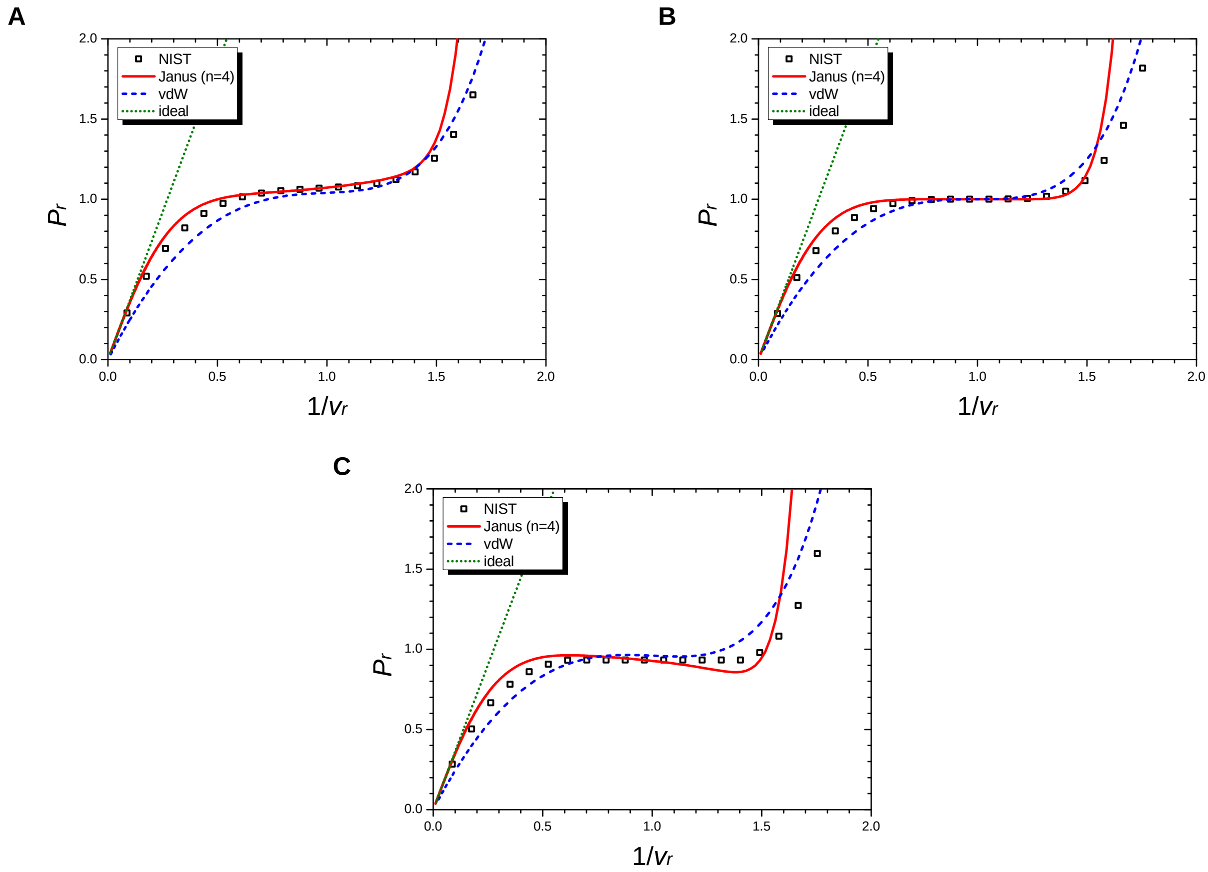

Figure S27. Isothermal curves of butane (C_4H_{10}) at $T_r = 1.01$ (**A**), $T_r = 1.00$ (**B**), and $T_r = 0.99$ (**C**). Boxes are from the NIST data. The red solid line is drawn from the $n = 4$ Janus van der Waals equation, the blue dashed line from the original van der Waals equation, and the green dotted line from the classical ideal gas law.

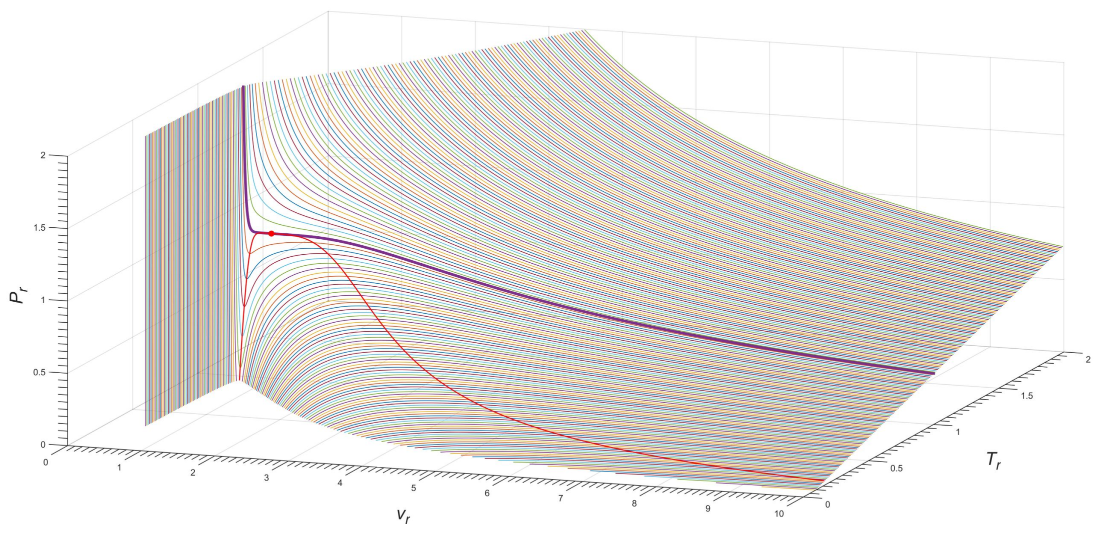

Figure S28. Three-dimensional $P_r - v_r - T_r$ phase diagram of the exact $n = 4$ Janus van der Waals equation, as for butane ($\mathrm{C_4H_{10}}$). The bold purple line corresponds to the isotherm of $T_r = 1.00$ as depicted in **Figure S27 B**; the red line is the Janus van der Waals spinodal curve with $a = 0.99$; and the red dot is the critical point.

1.8 isobutane (C_4H_{10})

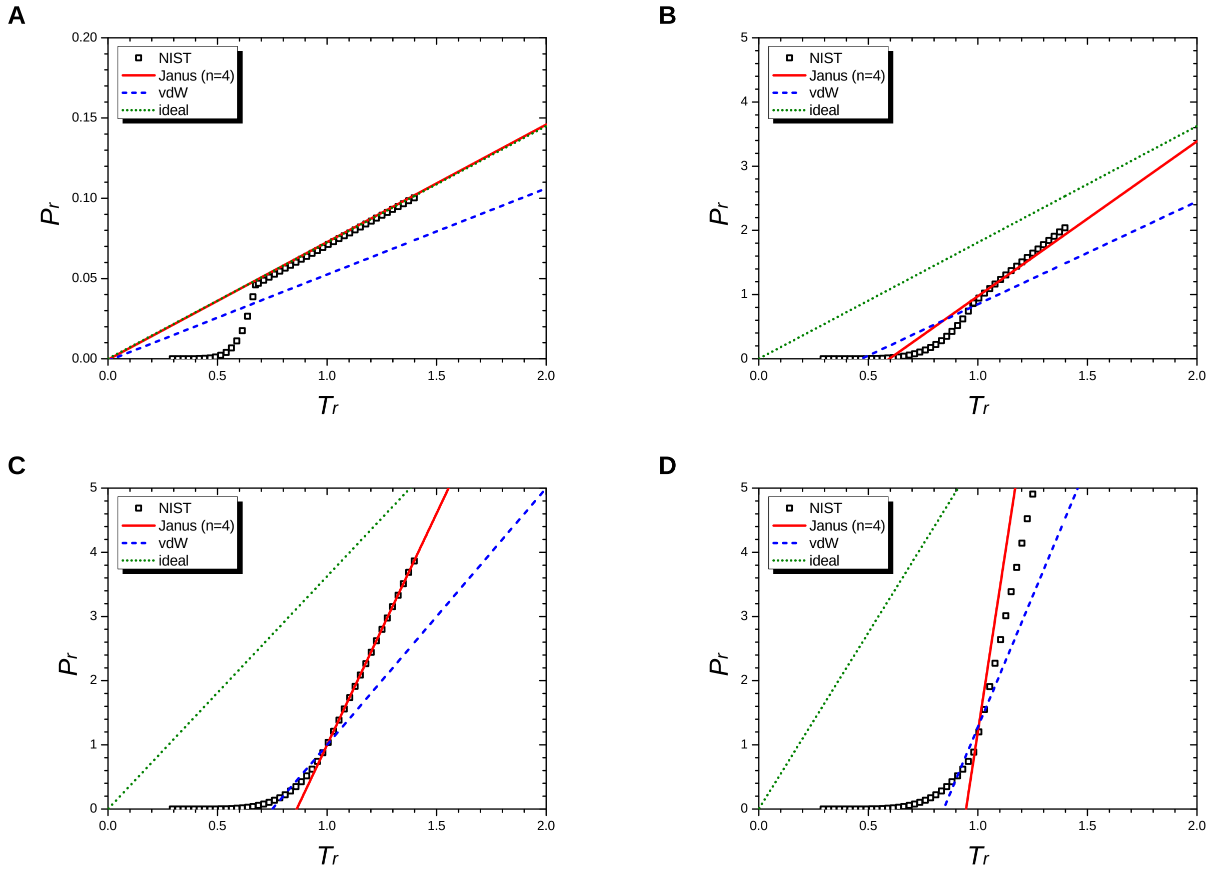

Figure S29. Isochoric curves of isobutane (C_4H_{10}) at $1/v_r = 0.02$ (**A**), $1/v_r = 0.5$ (**B**), $1/v_r = 1.0$ (**C**), and $1/v_r = 1.5$ (**D**). Boxes are from the NIST data. The red solid line is drawn from the $n = 4$ Janus van der Waals equation, the blue dashed line from the original van der Waals equation, and the green dotted line from the classical ideal gas law.

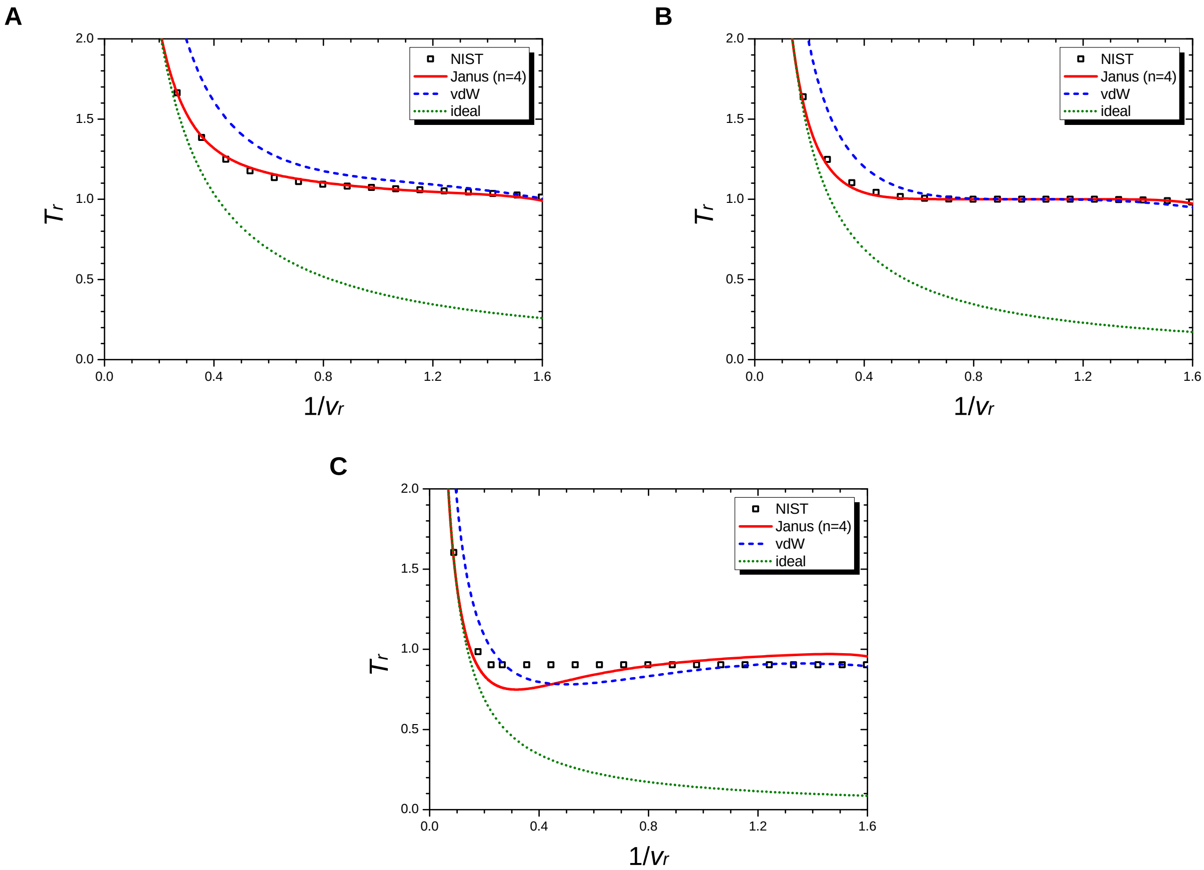

Figure S30. Isobaric curves of isobutane (C_4H_{10}) at $P_r = 1.5$ (**A**), $P_r = 1.0$ (**B**), and $P_r = 0.5$ (**C**). Boxes are from the NIST data. The red solid line is drawn from the $n = 4$ Janus van der Waals equation, the blue dashed line from the original van der Waals equation, and the green dotted line from the classical ideal gas law.

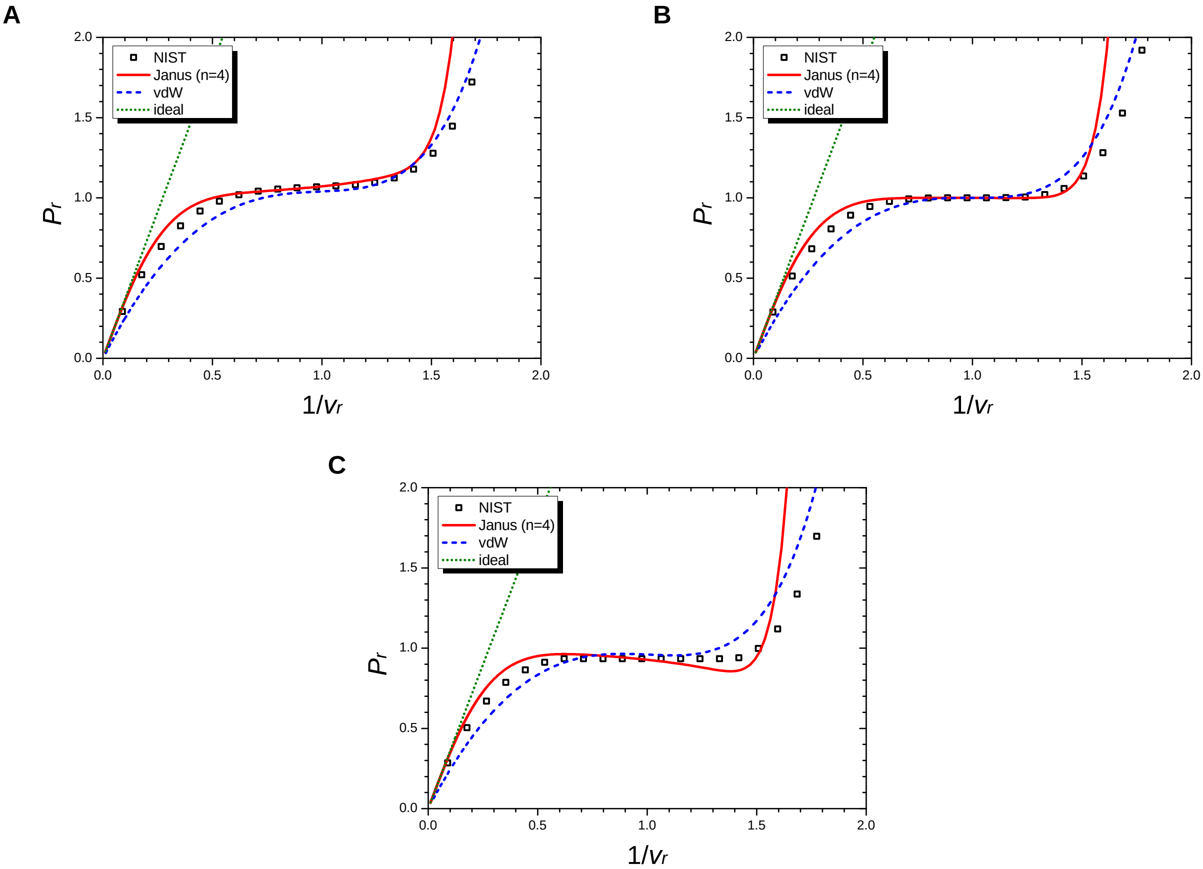

Figure S31. Isothermal curves of isobutane (C_4H_{10}) at $T_r = 1.01$ (**A**), $T_r = 1.00$ (**B**), and $T_r = 0.99$ (**C**). Boxes are from the NIST data. The red solid line is drawn from the $n = 4$ Janus van der Waals equation, the blue dashed line from the original van der Waals equation, and the green dotted line from the classical ideal gas law.

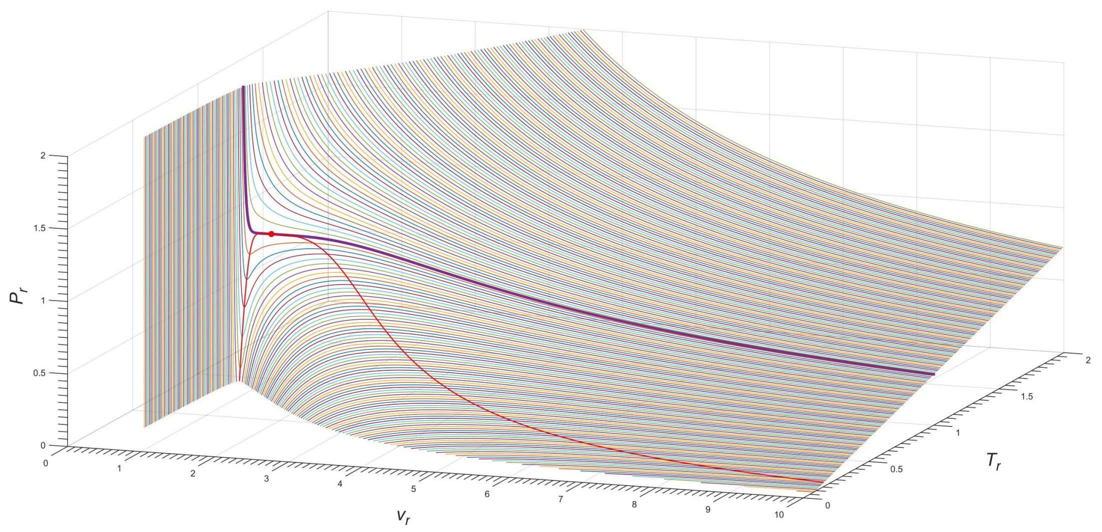

Figure S32. Three-dimensional $P_r - v_r - T_r$ phase diagram of the exact $n = 4$ Janus van der Waals equation, as for isobutane (C_4H_{10}). The bold purple line corresponds to the isotherm of $T_r = 1.00$ as depicted in **Figure S31 B**; the red line is the Janus van der Waals spinodal curve with $a = 0.99$; and the red dot is the critical point.

2 SUPPLEMENTARY FIGURES FOR $N = 6$ CASE

helium-4 (^{4}He)

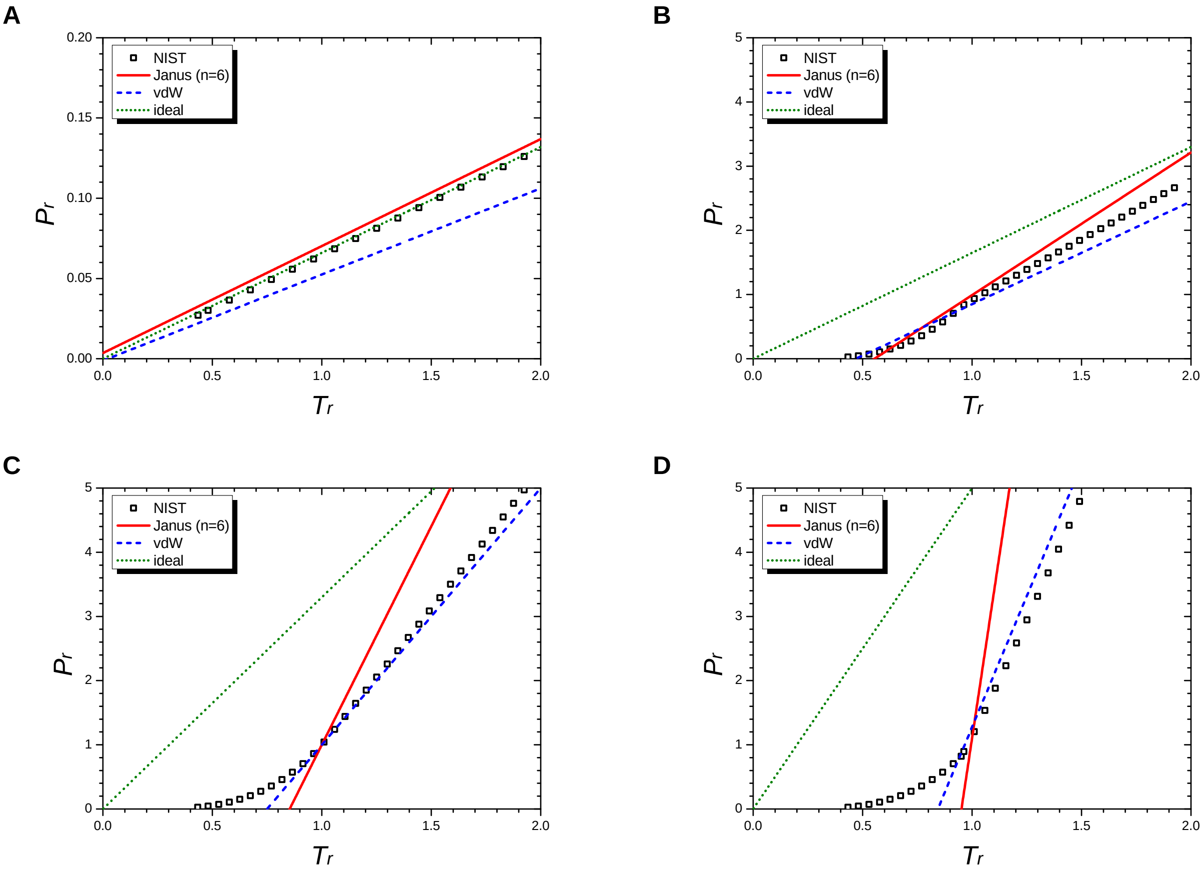

Figure S33. Isochoric curves of helium-4 (^{4}He) at $1/v_r = 0.02$ (**A**), $1/v_r = 0.5$ (**B**), $1/v_r = 1.0$ (**C**), and $1/v_r = 1.5$ (**D**). Boxes are from the NIST data. The red solid line is drawn from the $n = 6$ Janus van der Waals equation, the blue dashed line from the original van der Waals equation, and the green dotted line from the classical ideal gas law.

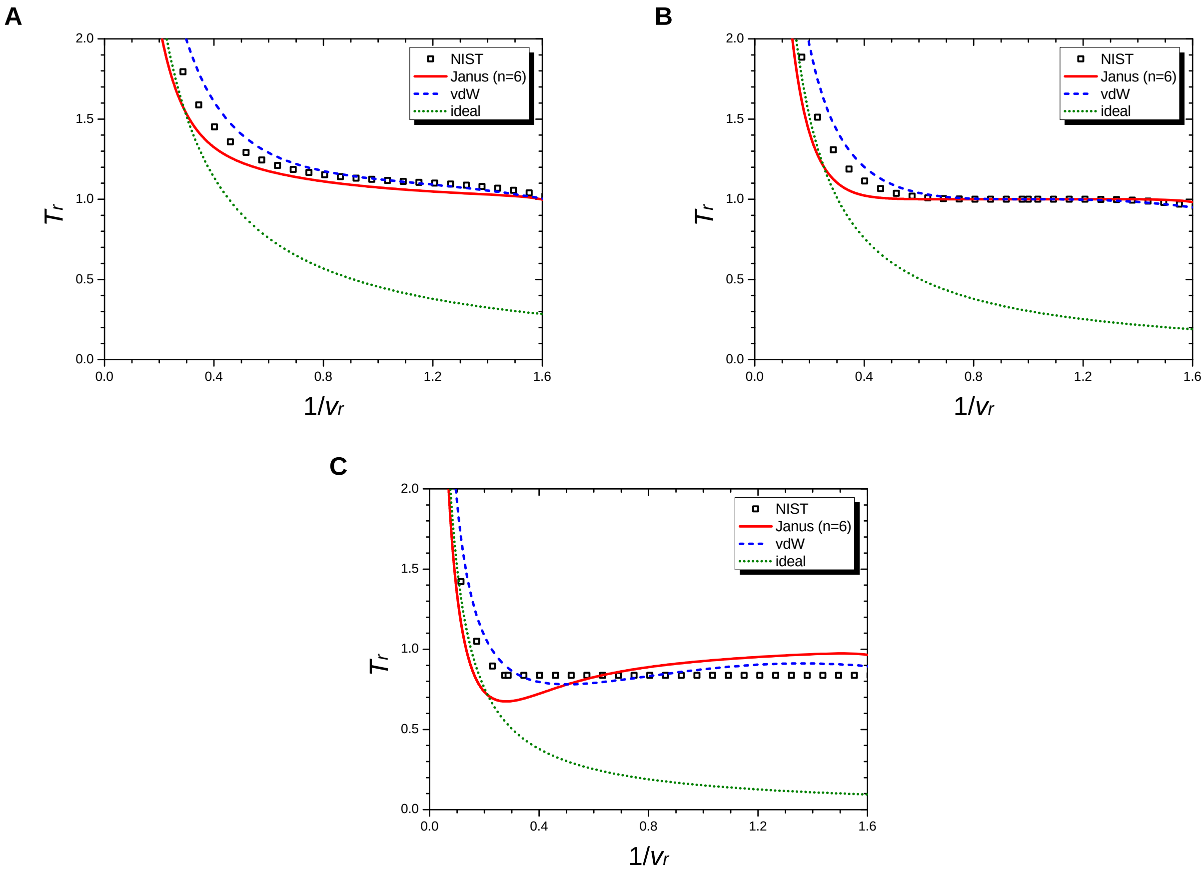

Figure S34. Isobaric curves of helium-4 (^{4}He) at $P_r = 1.5$ (**A**), $P_r = 1.0$ (**B**), and $P_r = 0.5$ (**C**). Boxes are from the NIST data. The red solid line is drawn from the $n = 6$ Janus van der Waals equation, the blue dashed line from the original van der Waals equation, and the green dotted line from the classical ideal gas law.

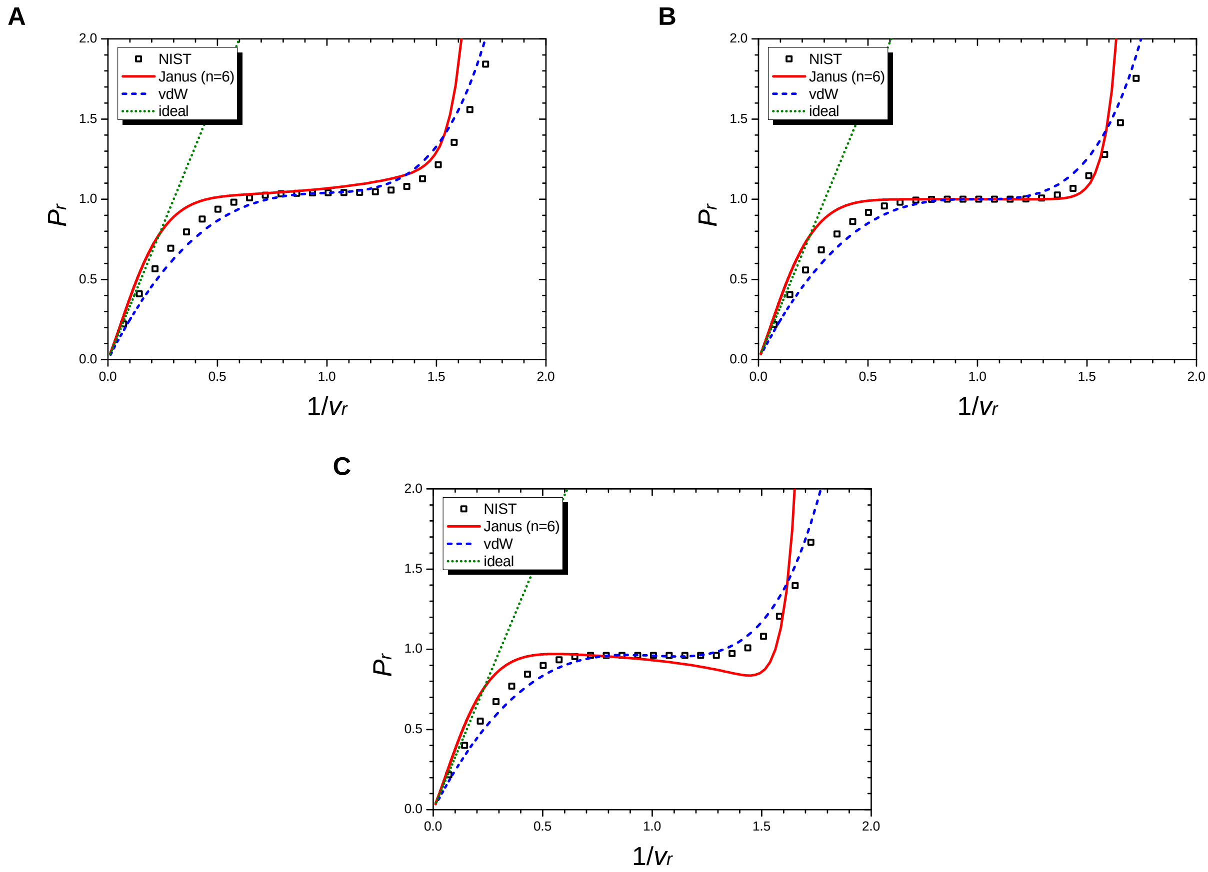

Figure S35. Isothermal curves of helium-4 (^{4}He) at $T_r = 1.01$ (**A**), $T_r = 1.00$ (**B**), and $T_r = 0.99$ (**C**). Boxes are from the NIST data. The red solid line is drawn from the $n = 6$ Janus van der Waals equation, the blue dashed line from the original van der Waals equation, and the green dotted line from the classical ideal gas law.

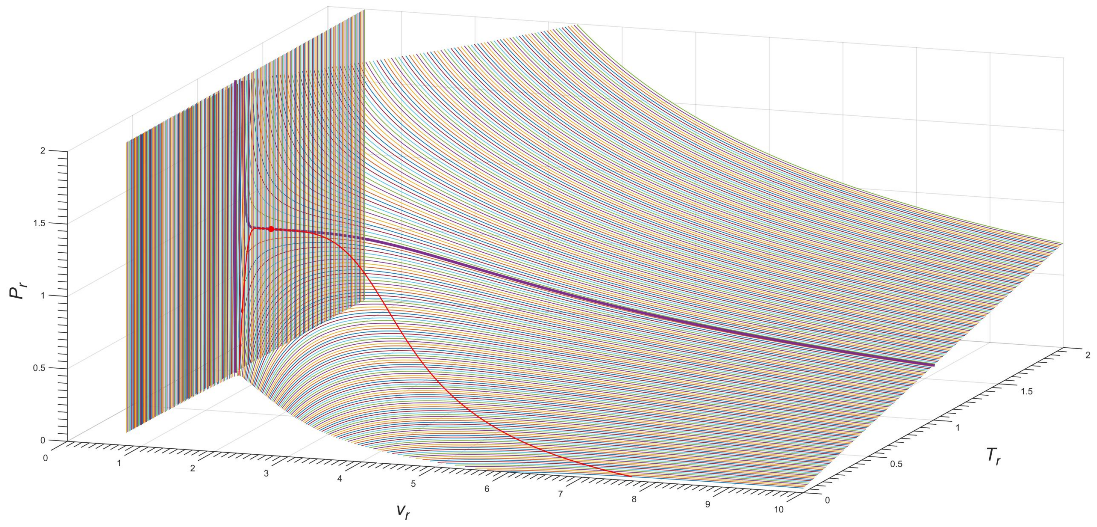

Figure S36. Three-dimensional $P_r - v_r - T_r$ phase diagram of the exact $n = 6$ Janus van der Waals equation, as for helium-4 ($^4\mathrm{He}$). The bold purple line corresponds to the isotherm of $T_r = 1.00$ as depicted in **Figure S35 B**; the red line is the Janus van der Waals spinodal curve with $a = 0.99$; and the red dot is the critical point.