

# Supporting Information: Effects of impurity gases on interfaces of the hydrogen-water-decane three-phase system: A square gradient theory investigation

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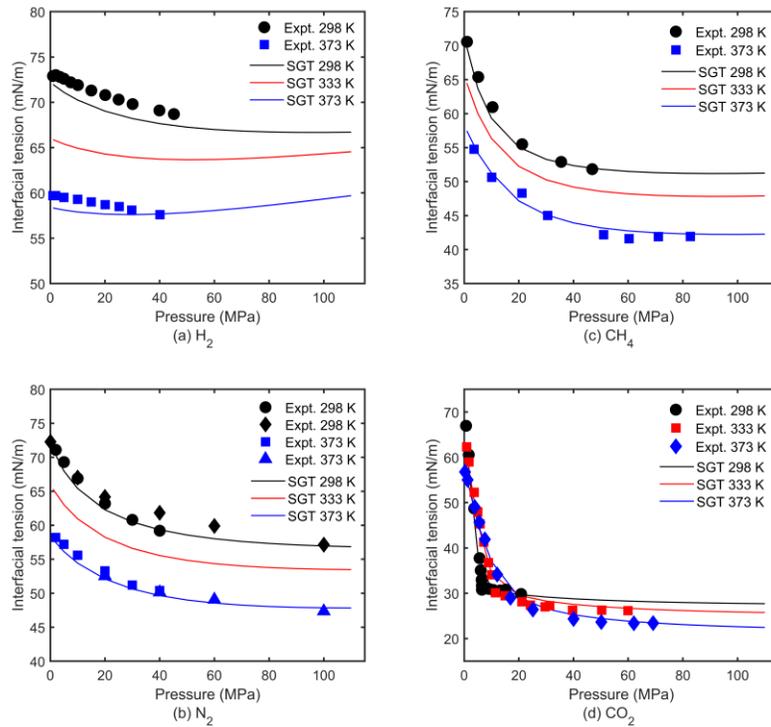
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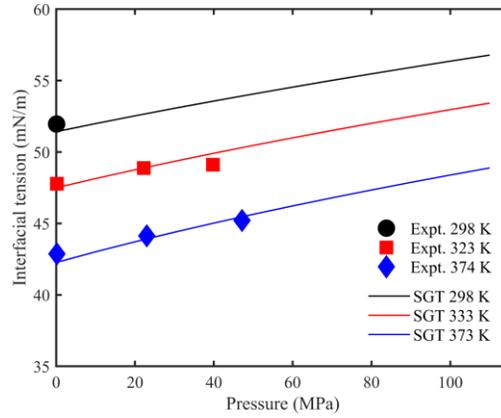
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## Appendix A.

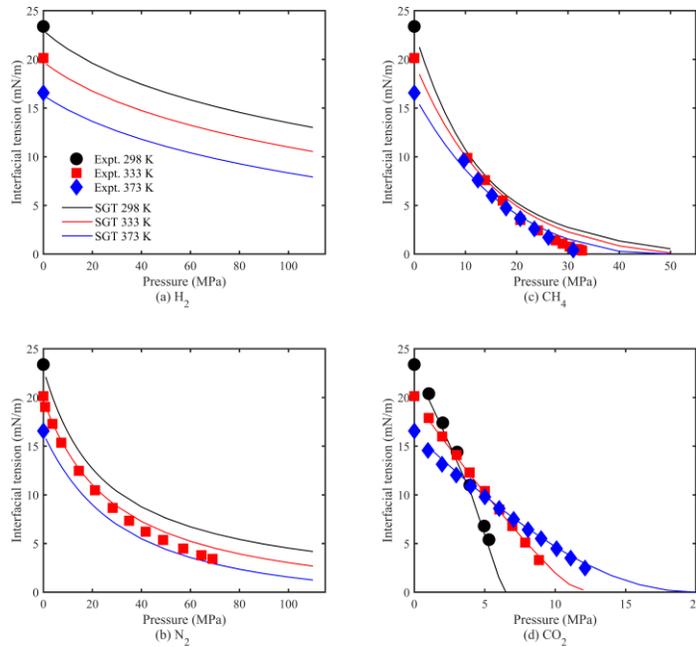


**Fig. A1** Pressure dependence of IFT in the gas-H<sub>2</sub>O 2-phase systems: (a) H<sub>2</sub>, (b) N<sub>2</sub>, (c) CH<sub>4</sub>, and (d) CO<sub>2</sub> at various temperatures. Predictions from SGT are shown as lines and the experimental data from Refs. S1-S7 are

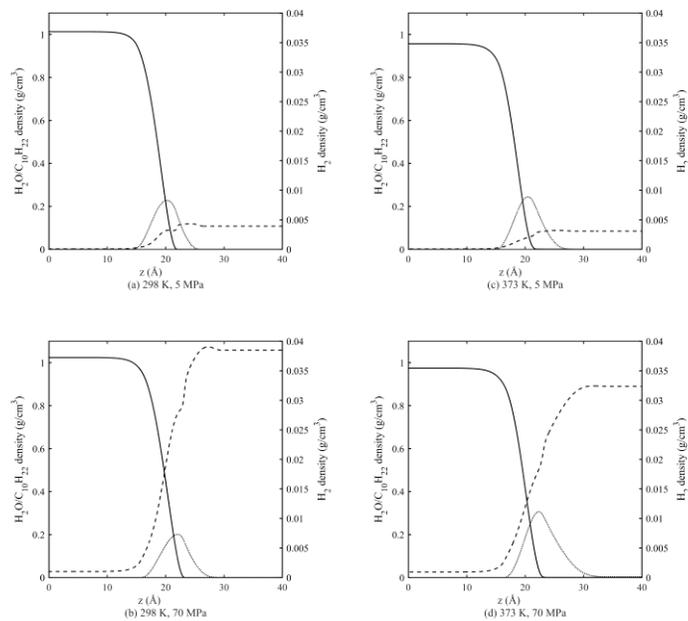
shown as filled symbols.



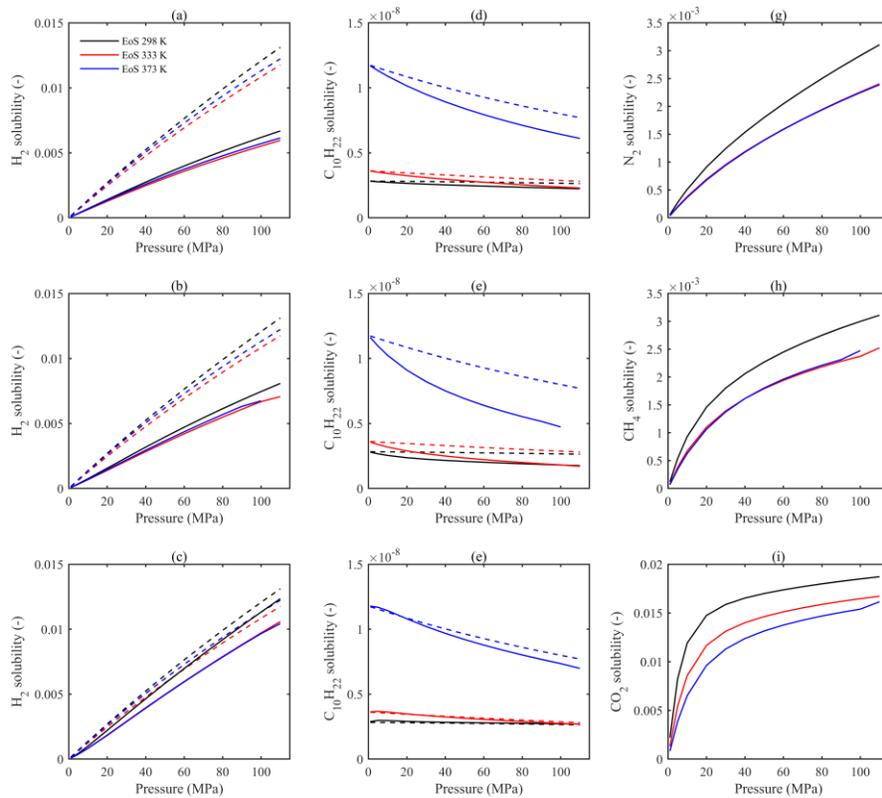
**Fig. A2** Pressure dependence of IFT in the H<sub>2</sub>O-decane 2-phase systems at various temperatures. Predictions from SGT are shown as lines and the experimental data from Ref. S8 are shown as filled symbols.



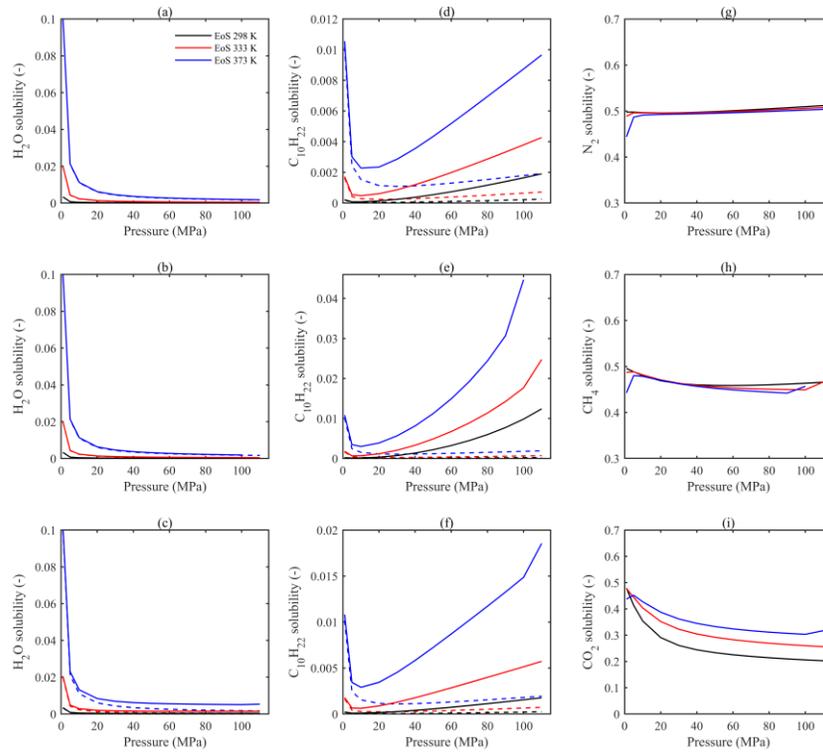
**Fig. A3** Pressure dependence of IFT in the gas-decane 2-phase systems: (a) H<sub>2</sub>, (b) N<sub>2</sub>, (c) CH<sub>4</sub>, and (d) CO<sub>2</sub> at various temperatures. Predictions from SGT are shown as lines and the experimental data from Refs. S9-S14 are shown as filled symbols.



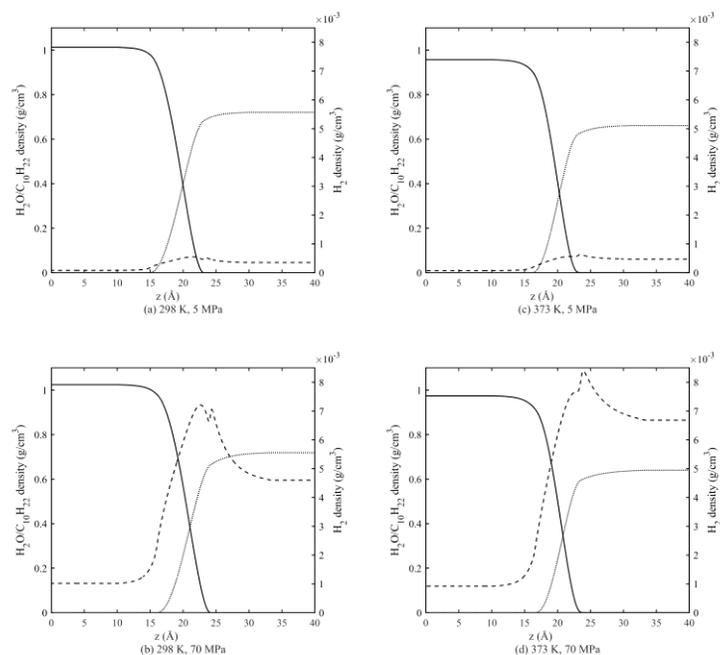
**Fig. A4** Equilibrium distributions of different species in the  $\text{H}_2$ - $\text{H}_2\text{O}$ - $\text{C}_{10}\text{H}_{22}$  3-phase system for the interface between  $\text{H}_2\text{O}$ -rich phase and  $\text{H}_2$ -rich phase at (a) 298 K, 5 MPa, (b) 298 K, 70 MPa, (c) 373 K, 5 MPa, and (d) 373 K, 70 MPa. The solid, dotted, and dashed lines denote  $\text{H}_2\text{O}$ , decane, and  $\text{H}_2$ , respectively. The data are taken from Ref. S15.



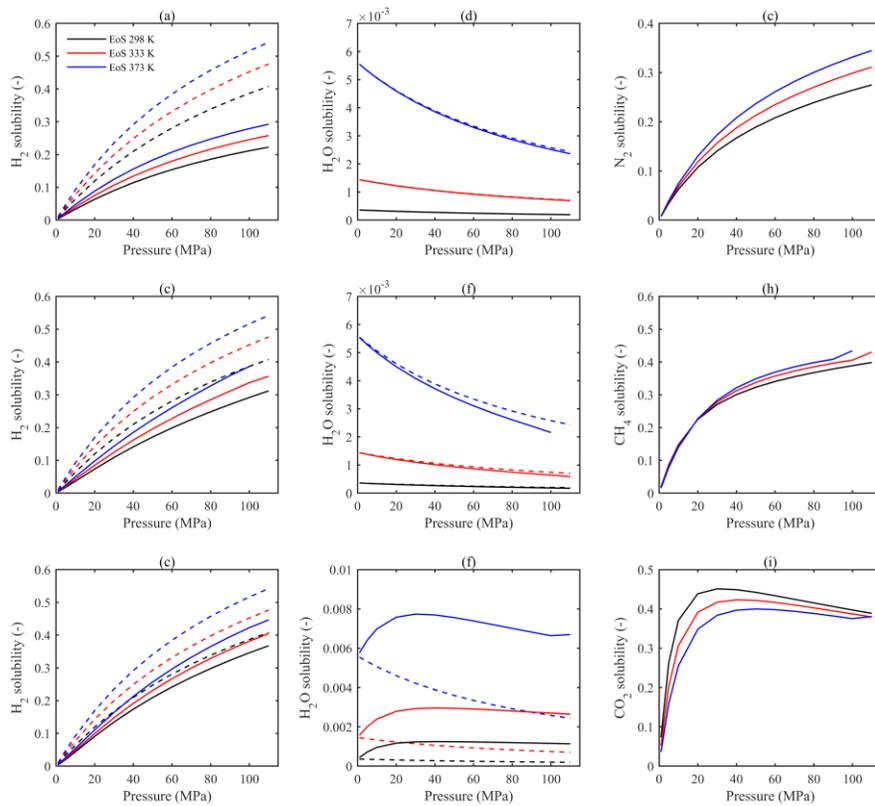
**Fig. A5** Solubilities in the H<sub>2</sub>O-rich phase in gas-H<sub>2</sub>-H<sub>2</sub>O-C<sub>10</sub>H<sub>22</sub> 3-phase systems. Top, middle, and bottom panels show solubilities in systems containing N<sub>2</sub>, CH<sub>4</sub>, and CO<sub>2</sub>, respectively. The data for dashed lines are taken from Ref. S15.



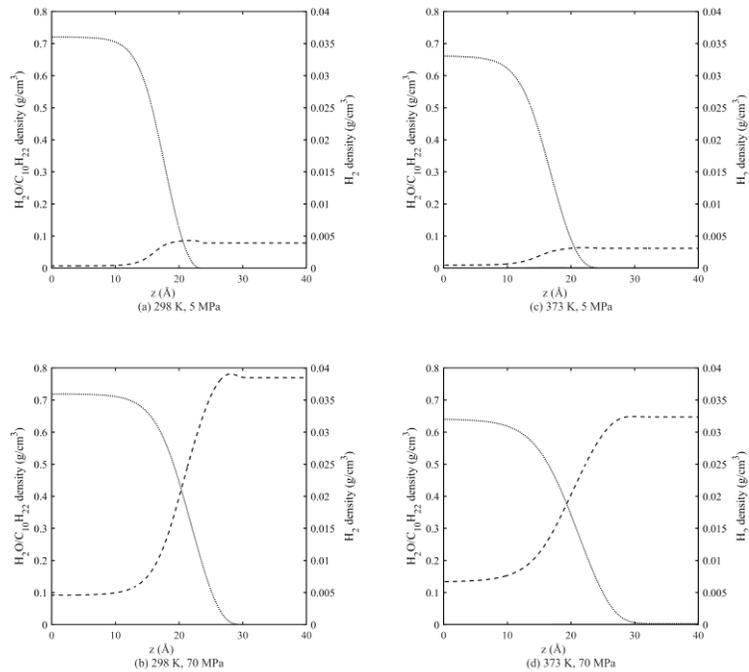
**Fig. A6** Solubilities in the  $H_2$ -rich phase in gas- $H_2$ - $H_2O$ - $C_{10}H_{22}$  3-phase systems. Top, middle, and bottom panels show solubilities in systems containing  $N_2$ ,  $CH_4$ , and  $CO_2$ , respectively. The data for dashed lines are taken from Ref. S15.



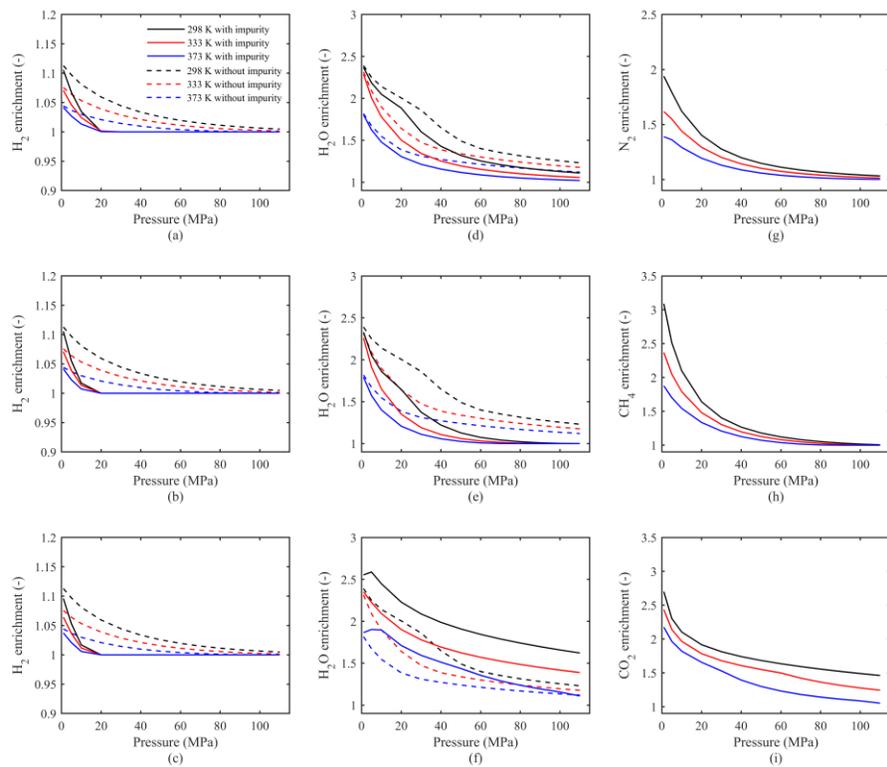
**Fig. A7** Equilibrium distributions of different species in the  $\text{H}_2\text{-H}_2\text{O-C}_{10}\text{H}_{22}$  3-phase system for the interface between  $\text{H}_2\text{O}$ -rich phase and  $\text{C}_{10}\text{H}_{22}$ -rich phase at (a) 298 K, 5 MPa, (b) 298 K, 70 MPa, (c) 373 K, 5 MPa, and (d) 373 K, 70 MPa. The solid, dotted, and dashed lines denote  $\text{H}_2\text{O}$ , decane, and  $\text{H}_2$ , respectively. The data are taken from Ref. S15.



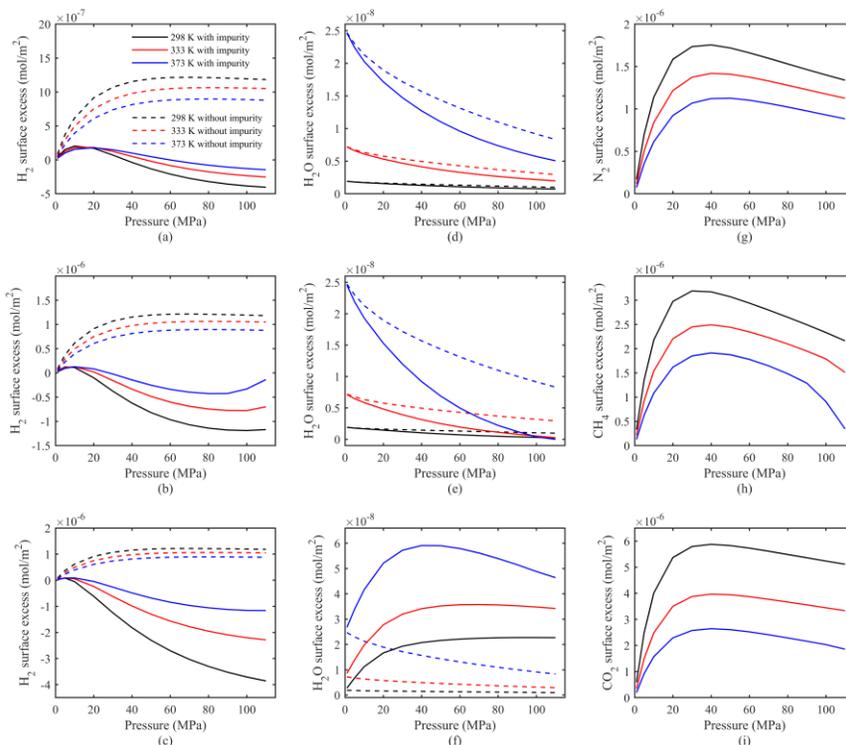
**Fig. A8** Solubilities in the  $C_{10}H_{22}$ -rich phase in gas- $H_2$ - $H_2O$ - $C_{10}H_{22}$  3-phase systems. Top, middle, and bottom panels show solubilities in systems containing  $N_2$ ,  $CH_4$ , and  $CO_2$ , respectively. The data for dashed lines are taken from Ref. S15.



**Fig. A9** Equilibrium distributions of different species in the  $\text{H}_2$ - $\text{H}_2\text{O}$ - $\text{C}_{10}\text{H}_{22}$  3-phase system for the interface between  $\text{H}_2$ -rich phase and  $\text{C}_{10}\text{H}_{22}$ -rich phase at (a) 298 K, 5 MPa, (b) 298 K, 70 MPa, (c) 373 K, 5 MPa, and (d) 373 K, 70 MPa. The solid, dotted, and dashed lines denote  $\text{H}_2\text{O}$ , decane, and  $\text{H}_2$ , respectively. The data are taken from Ref. S15.



**Fig. A10** Component enrichments of the H<sub>2</sub>-H<sub>2</sub>O-C<sub>10</sub>H<sub>22</sub> interface. Top, middle, and bottom panels show surface excesses in systems containing N<sub>2</sub>, CH<sub>4</sub>, and CO<sub>2</sub>, respectively. Dashed lines are taken from Ref. S15.



**Fig. A11** Component surface excesses of the  $\text{H}_2\text{-H}_2\text{O-C}_{10}\text{H}_{22}$  interface. Top, middle, and bottom panels show surface excesses in systems containing  $\text{N}_2$ ,  $\text{CH}_4$ , and  $\text{CO}_2$ , respectively. Dashed lines are taken from Ref. S15.

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