

Supporting Information:

**Prediction of Composition-Dependent Self-Diffusion
Coefficients in Binary Liquid Mixtures:
The Missing Link for Darken-Based Models**

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S1 Self-diffusion coefficients of Lennard-Jones (LJ) systems

S1.1 Relative deviations $\Delta D_{2,\text{self,rel}}$ of the McCarty-Mason prediction as a function of the thermodynamic factor Γ for component 2

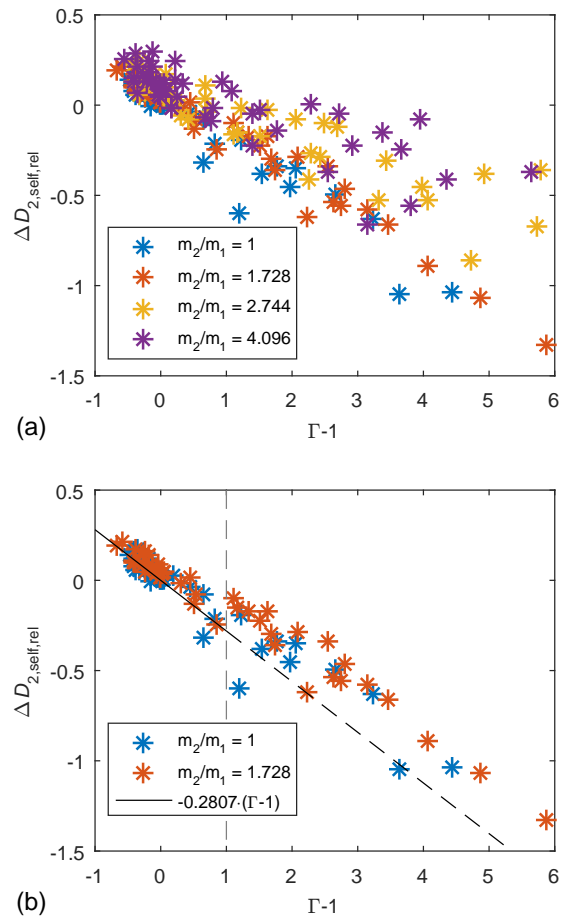


Figure S1: Relative deviations $\Delta D_{2,\text{self,rel}}$ of the McCarty-Mason prediction as function of the thermodynamic factor Γ for LJ systems.

(a) $\Delta D_{2,\text{self,rel}}$ for all LJ systems, differentiated by the molar mass ratios m_2/m_1 .

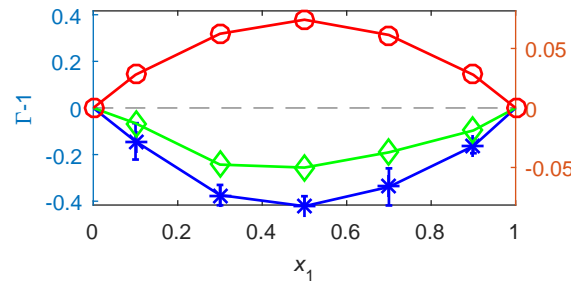
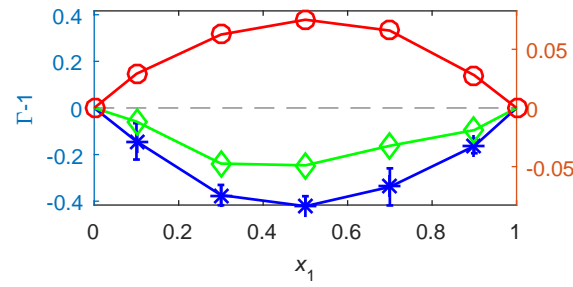
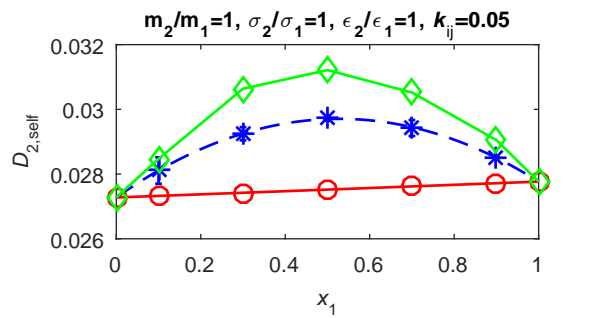
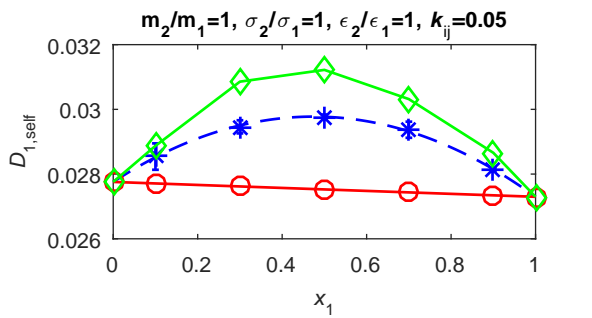
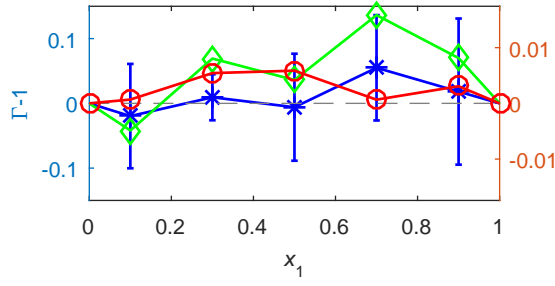
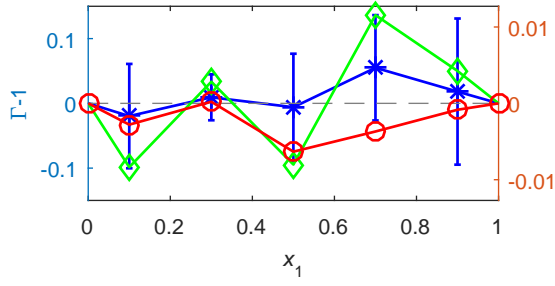
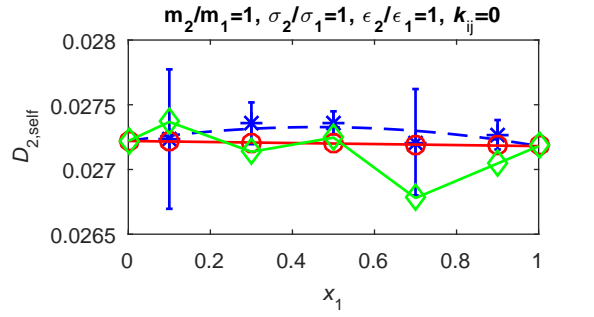
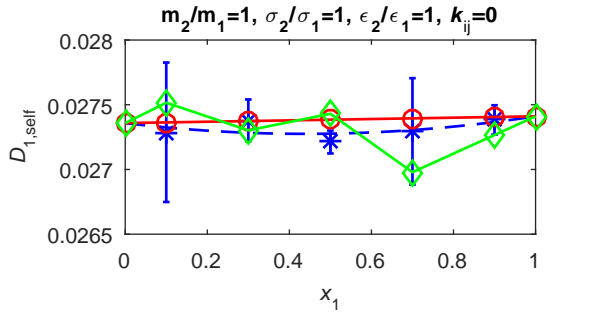
(b) $\Delta D_{2,\text{self,rel}}$ for LJ systems with molar mass ratios $m_2/m_1 < 2$ and best fit of Equation 15 (black line) for $0 < \Gamma < 2$ (indicated by the vertical dashed line).

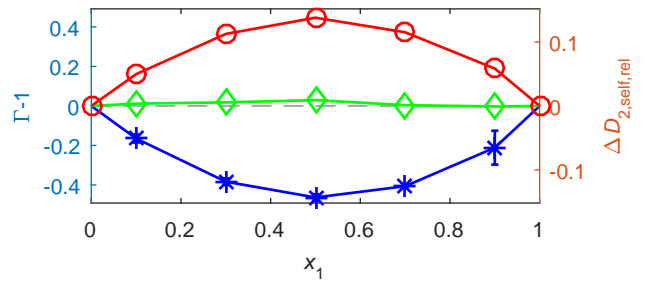
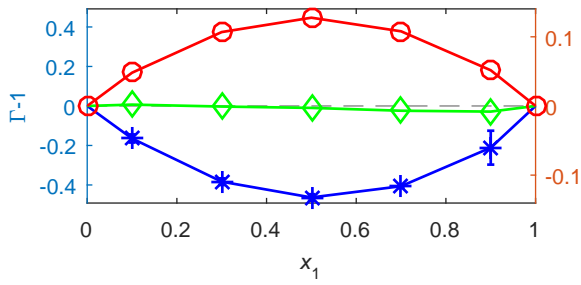
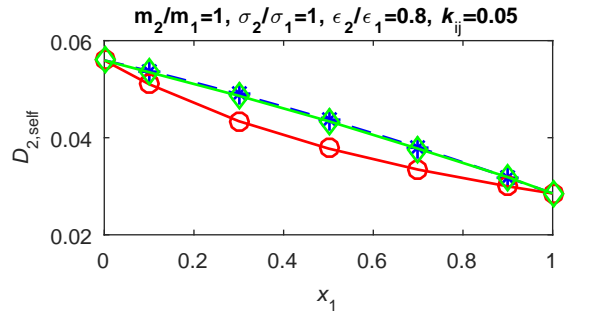
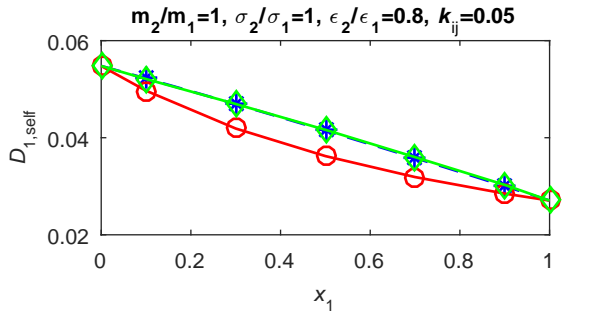
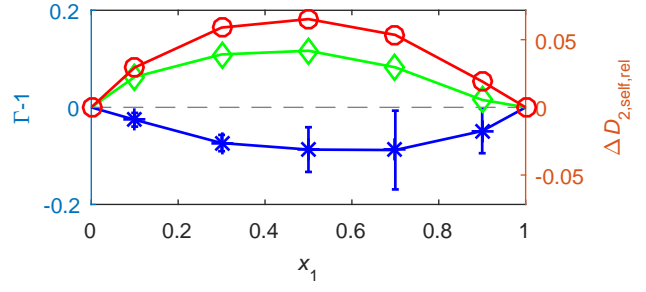
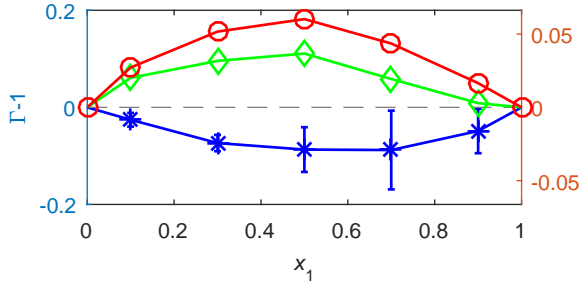
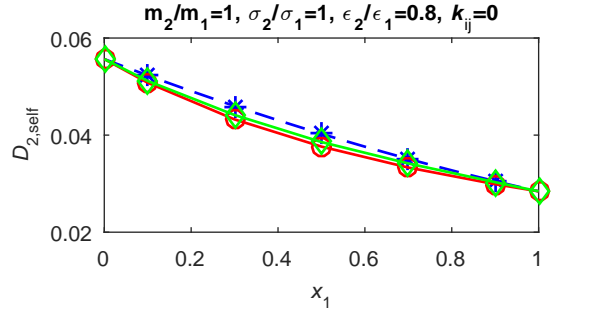
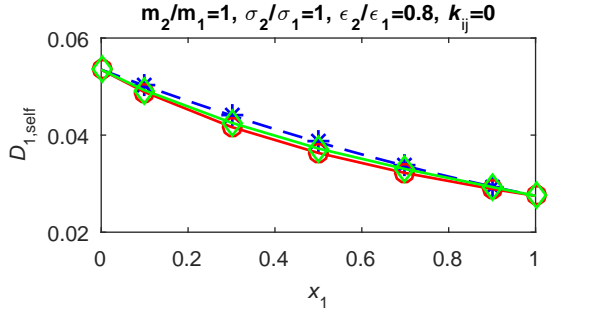
S1.2 LJ systems with molar mass ratios $m_2/m_1 < 2$

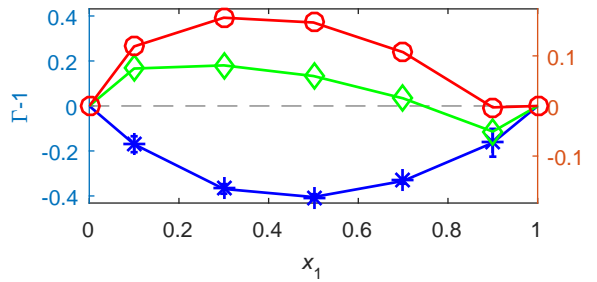
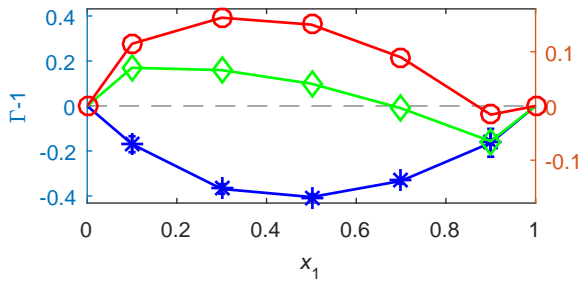
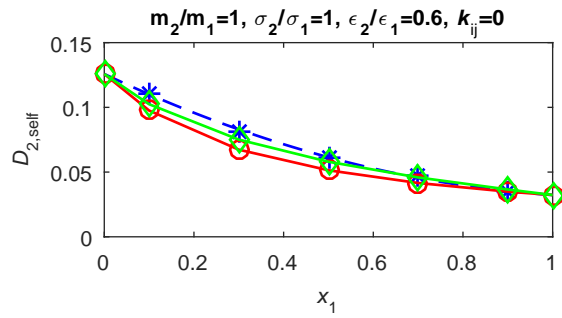
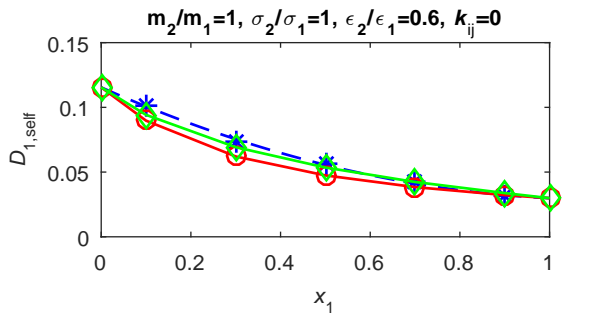
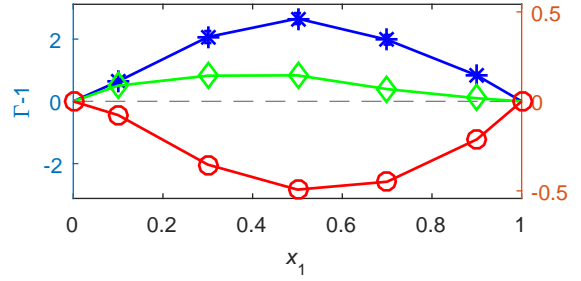
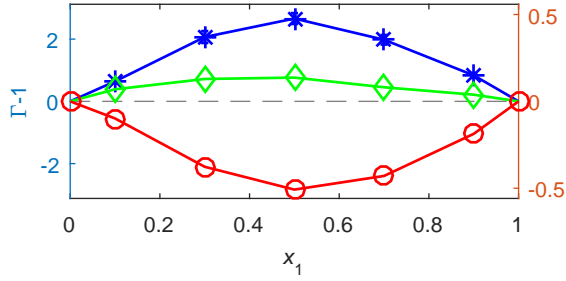
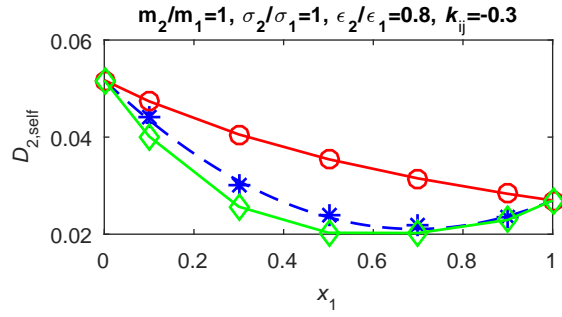
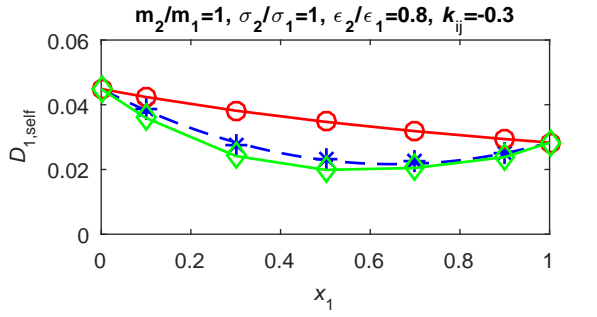
Composition-dependent self-diffusion coefficients $D_{i,\text{self}}$, thermodynamic factors $\Gamma - 1$, and relative deviations $\Delta D_{i,\text{self,rel}}$ of LJ systems with molar mass ratios $m_2/m_1 < 2$. The specifications of the LJ systems ϵ_2/ϵ_1 , σ_2/σ_1 , m_2/m_1 , and k_{ij} are given in the title of each figure.

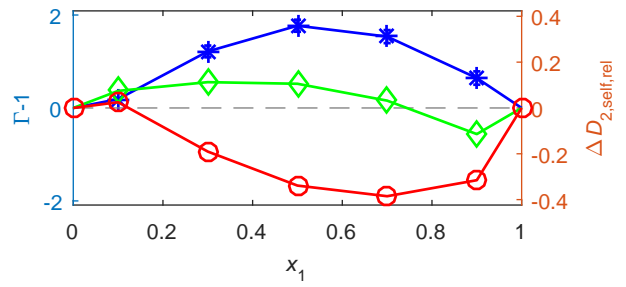
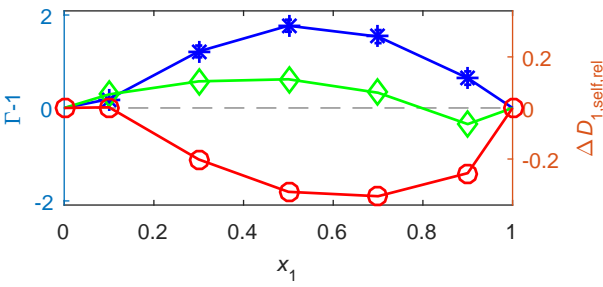
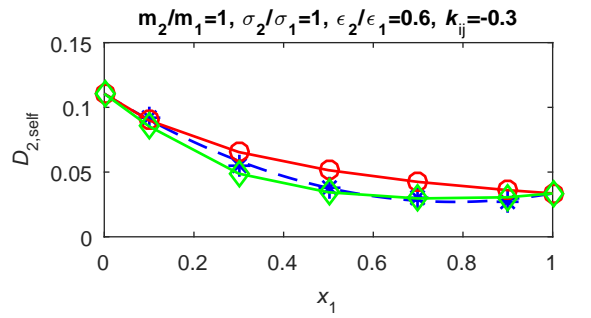
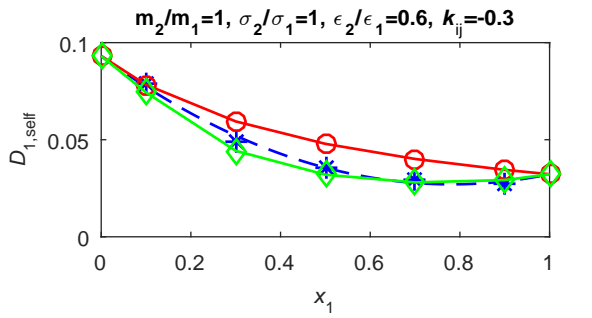
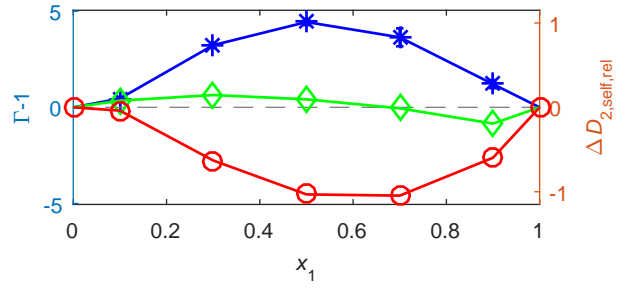
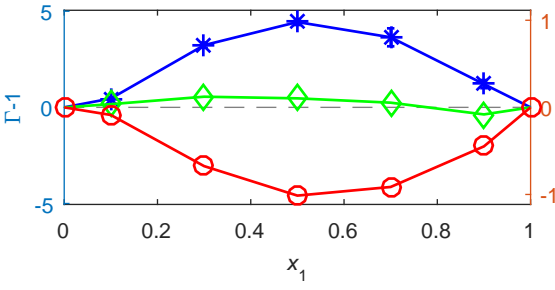
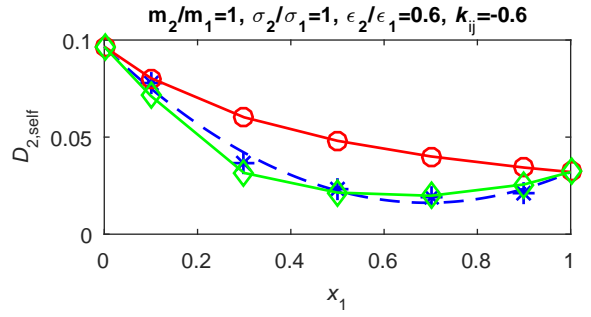
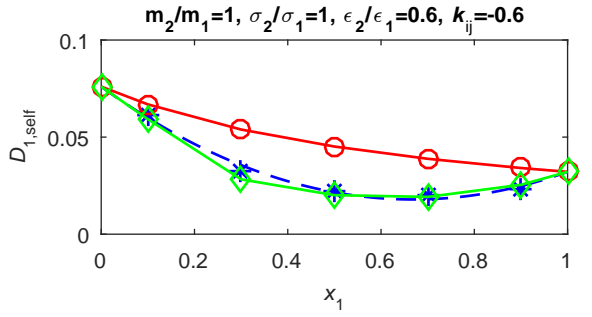
Top figures: Blue stars: Simulation results of self-diffusion coefficients $D_{i,\text{self}}$ of binary LJ systems as function of the mole fraction x_1 of the first species. Blue dashed line: smoothing fit to the simulation results; red circles/line: predictions of the McCarty-Mason equation (Equation 6); green diamonds/line: predictions of the modified McCarty-Mason equation (Equation 25). The error bars of $D_{i,\text{self}}$ are smaller than the symbols in most cases. Please note that y -axes are adapted for each system.

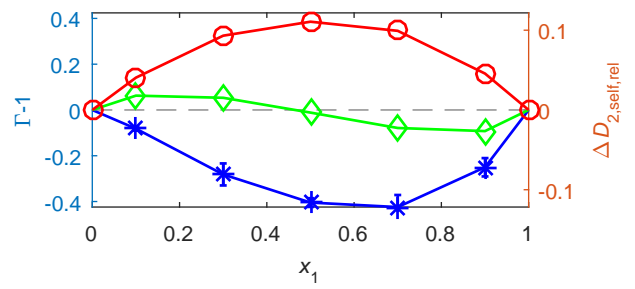
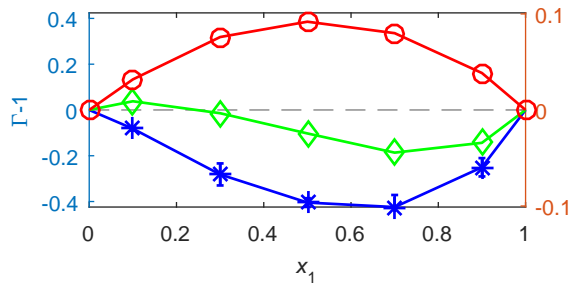
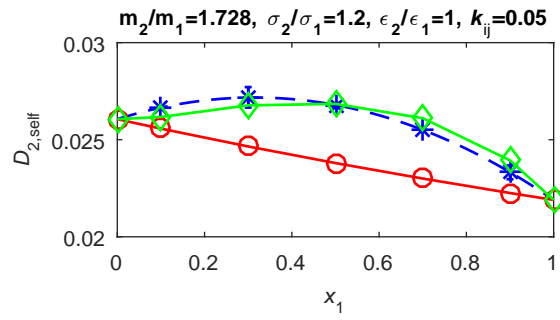
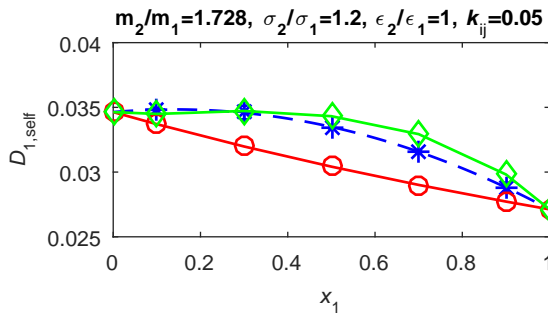
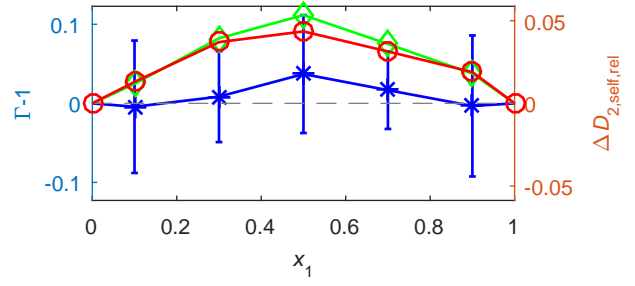
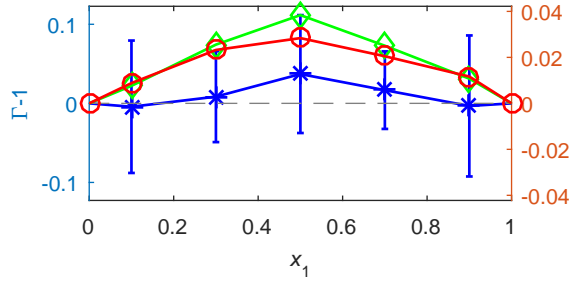
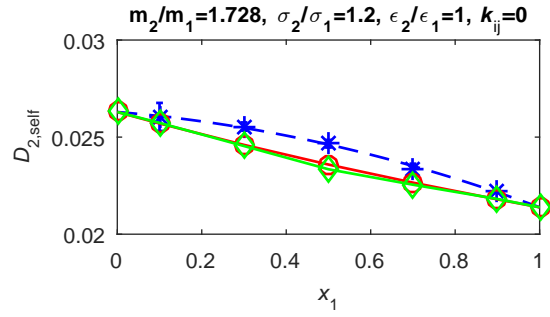
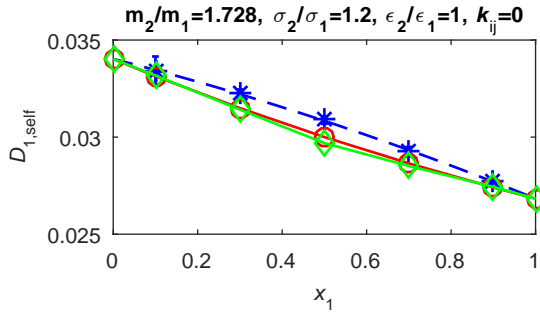
Bottom figures: Composition dependence of the thermodynamic factor $\Gamma - 1$ (blue stars/line, left axis) and composition dependence of the relative deviation $\Delta D_{i,\text{self,rel}}$ between the self-diffusion coefficients and the predictions of the McCarty-Mason equation (Equation 6) (red circles/line, right axis) and the modified McCarthy-Mason equation (Equation 25) (green diamonds/line, right axis). A clear correlation between $\Gamma - 1$ and $\Delta D_{i,\text{self,rel}}$ can be observed. The error bars of $\Gamma - 1$ are smaller than the symbols in most cases. Please note that y -axes are adapted for each system.

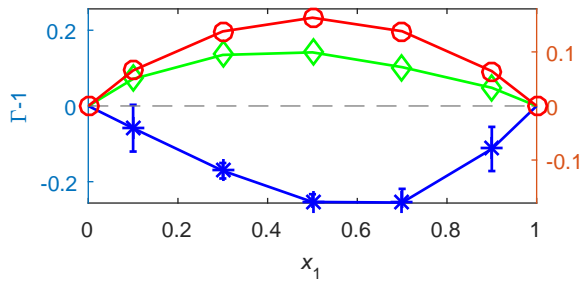
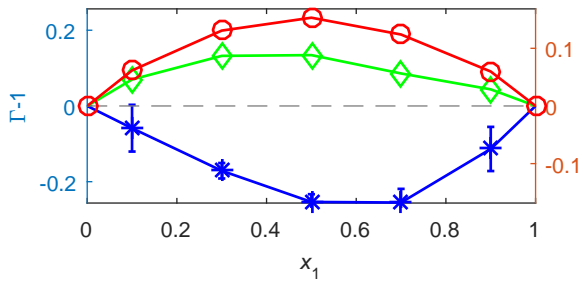
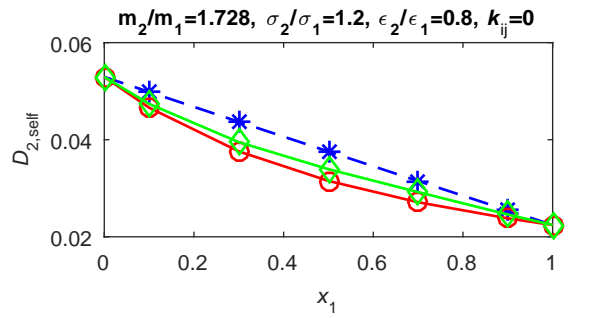
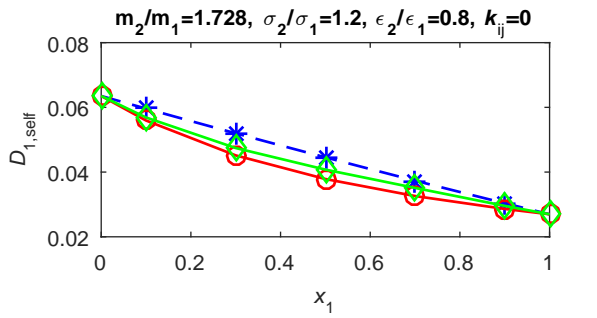
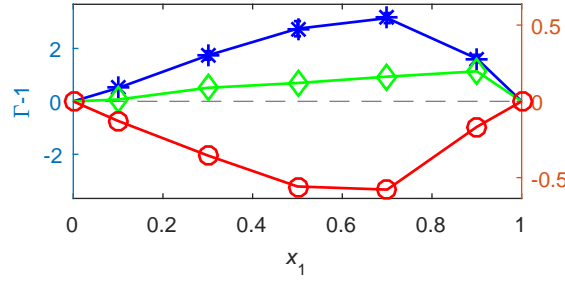
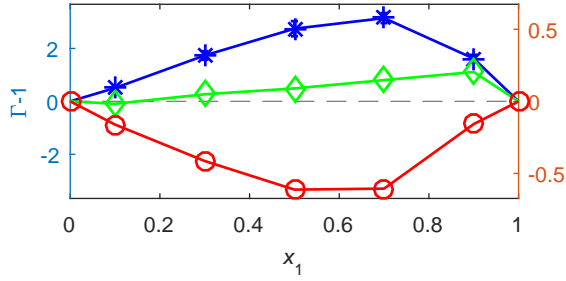
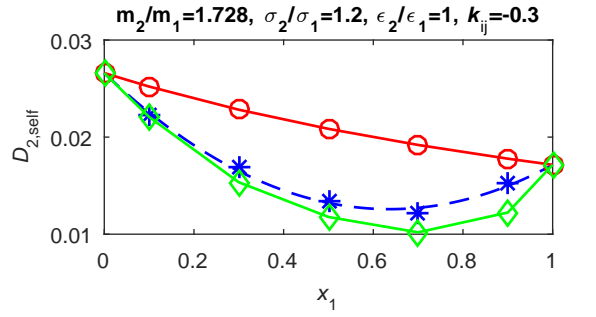
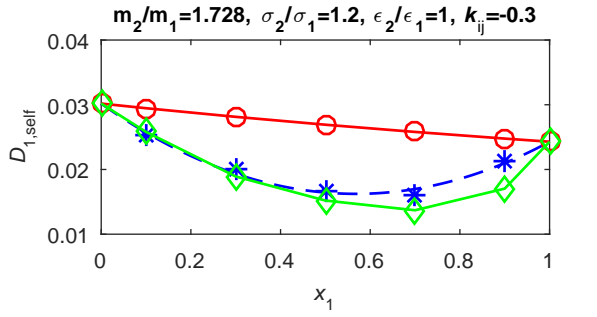


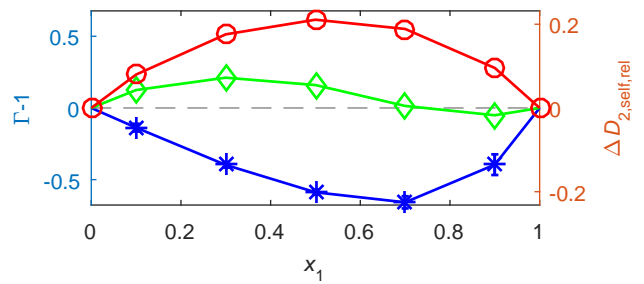
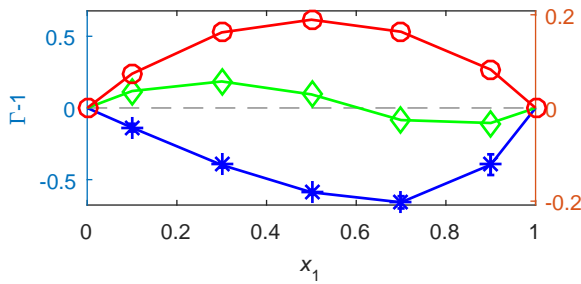
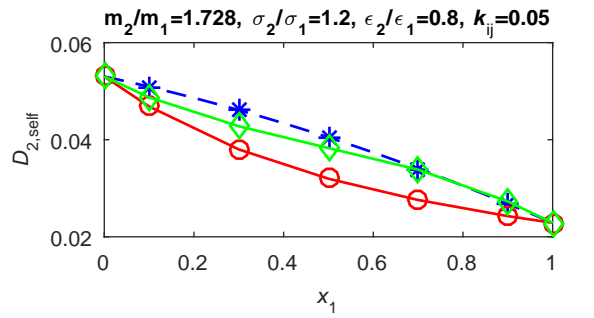
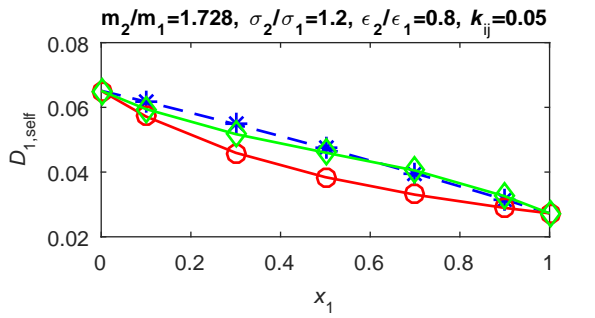
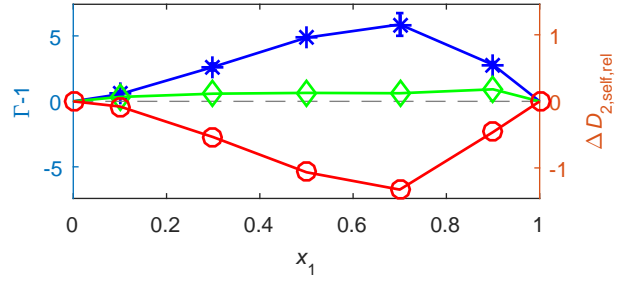
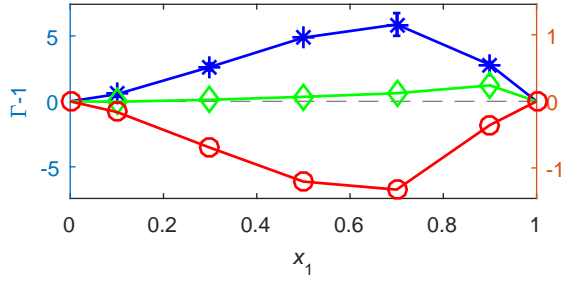
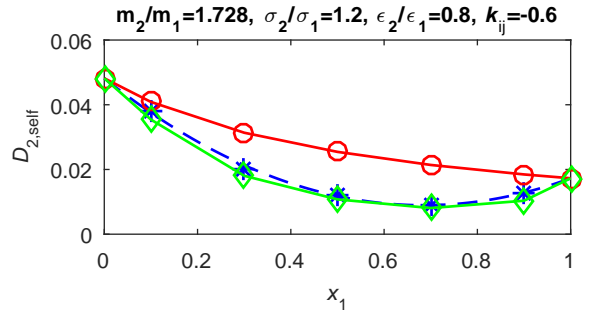
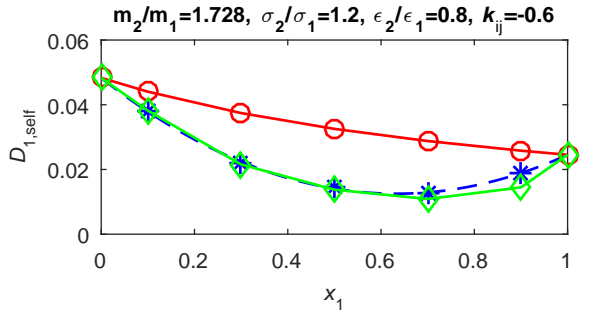


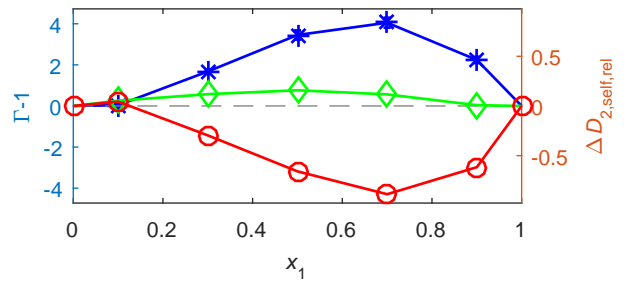
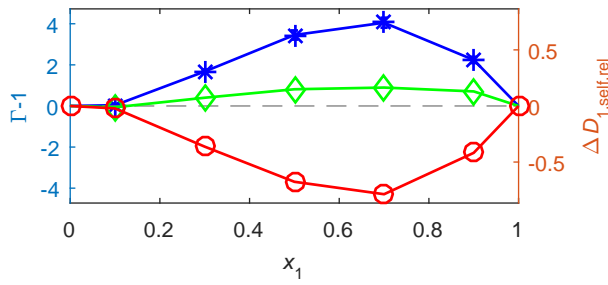
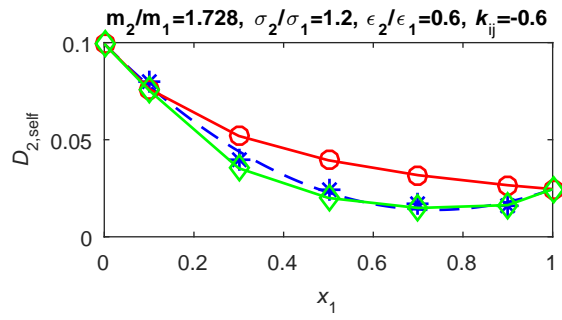
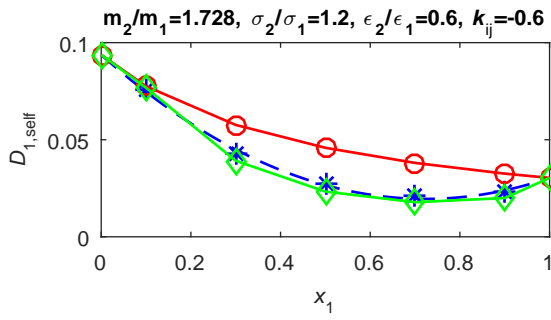
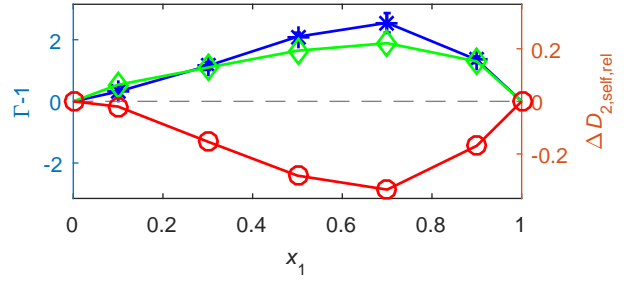
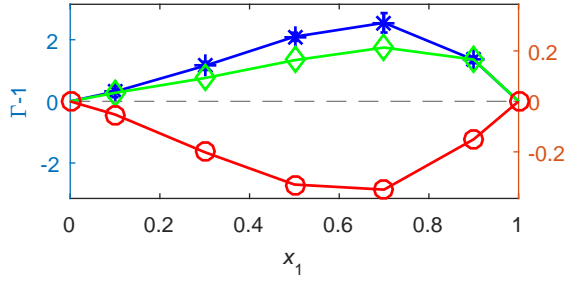
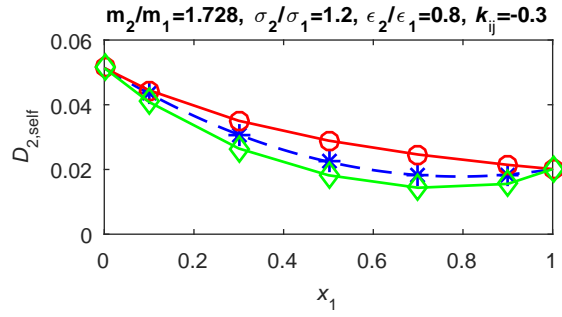
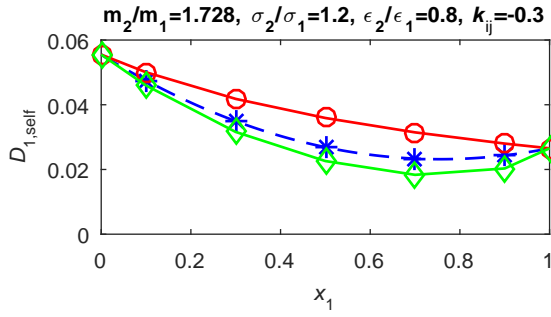


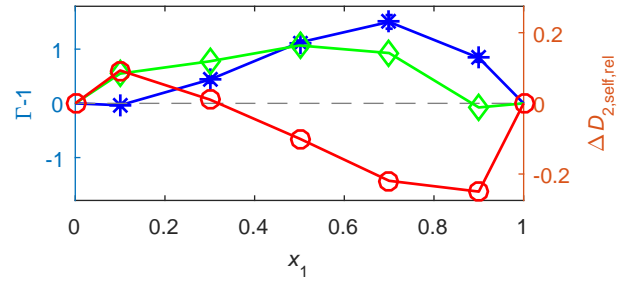
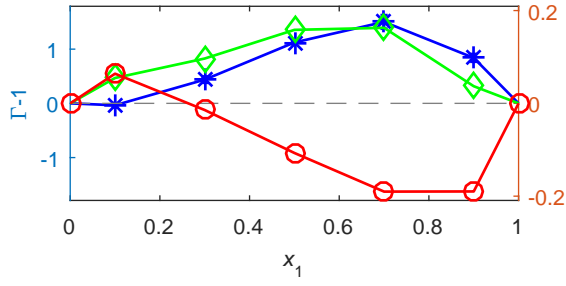
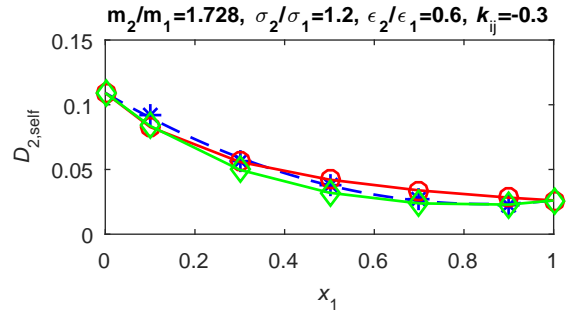
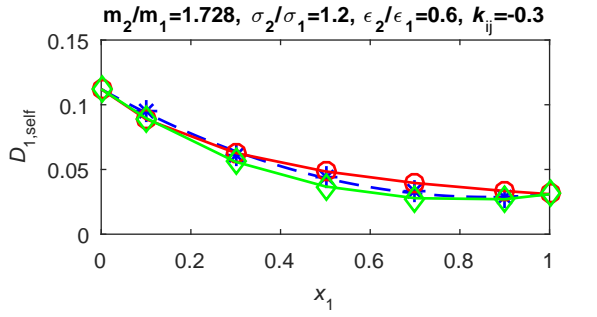










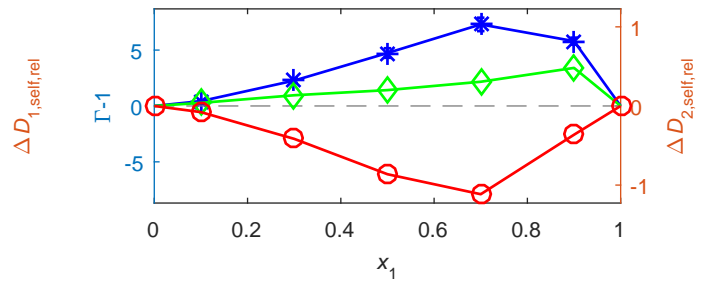
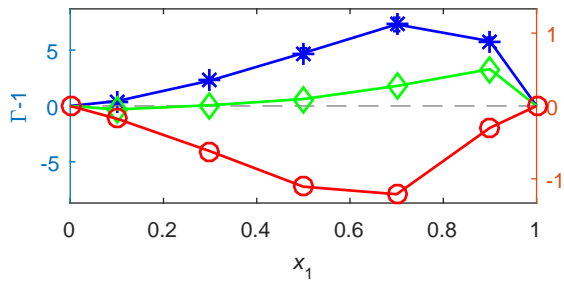
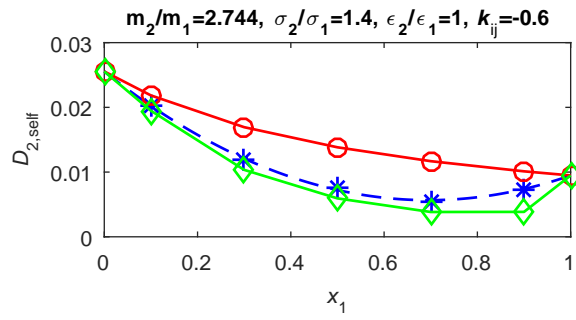
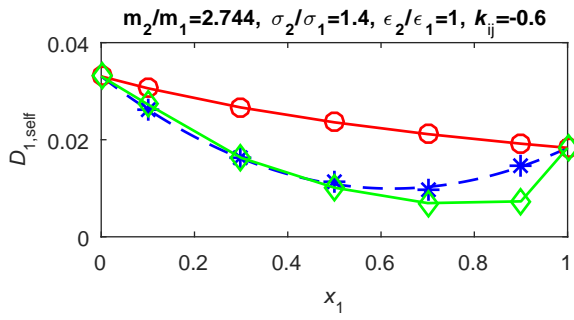
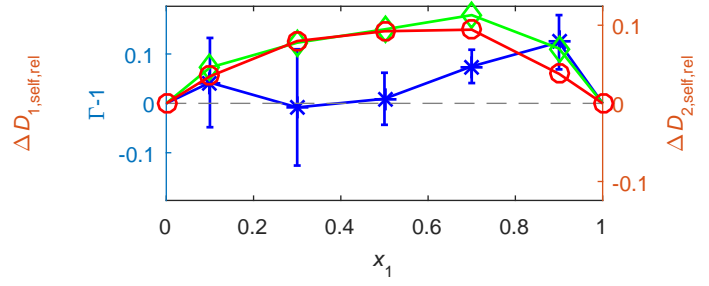
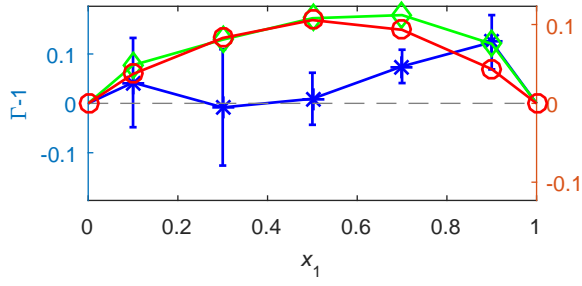
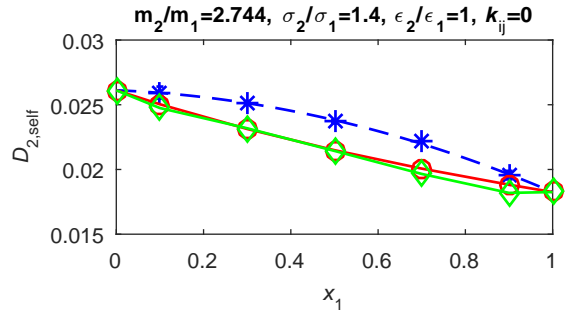
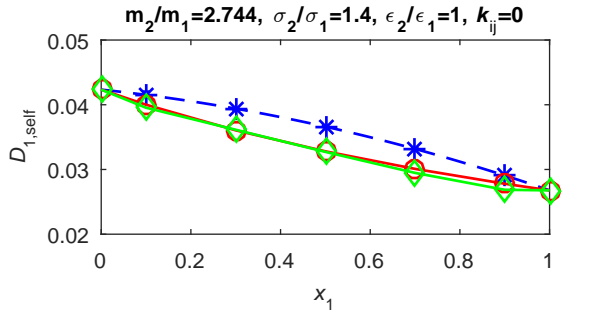


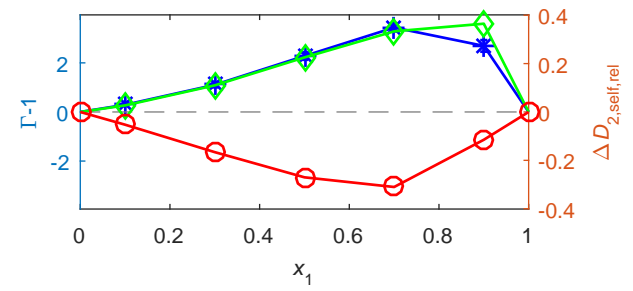
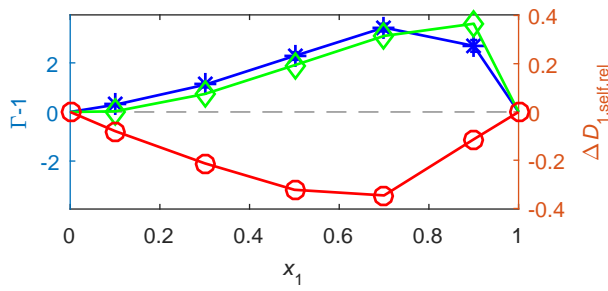
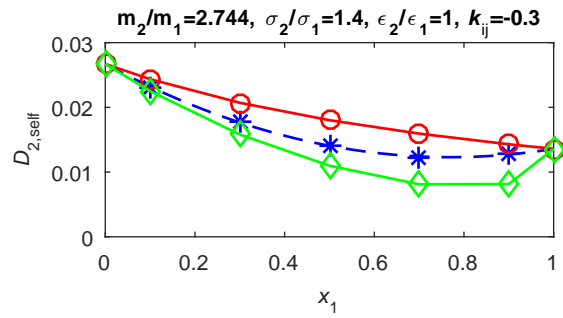
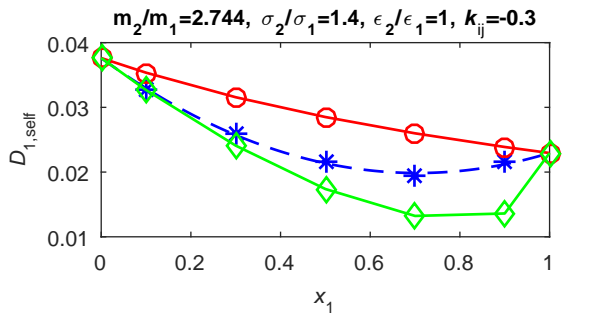
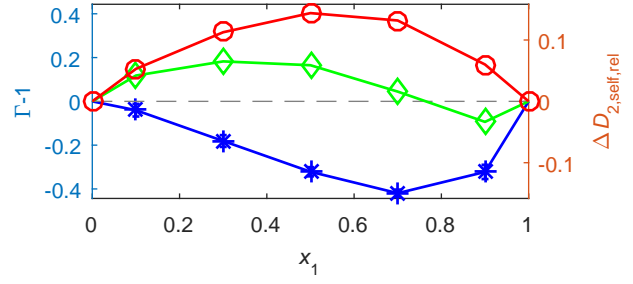
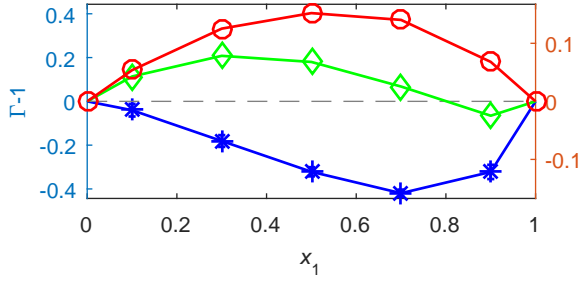
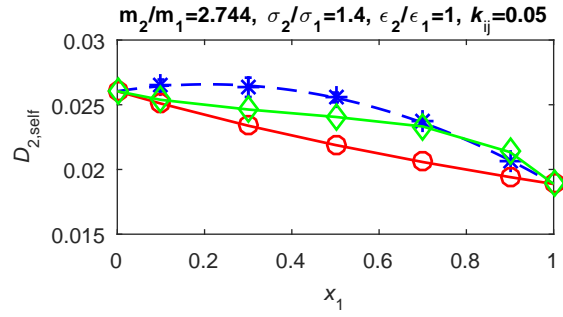
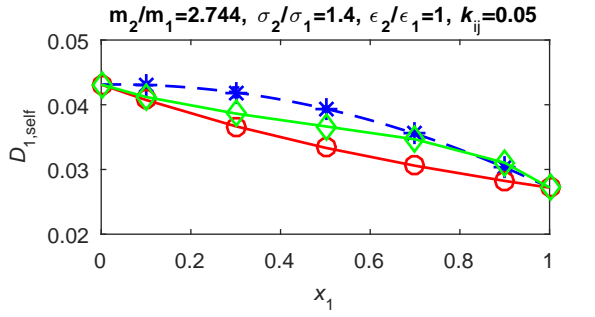
S1.3 LJ systems with molar mass ratios $m_2/m_1 > 2$

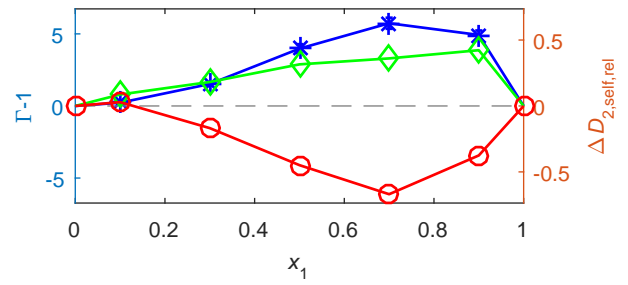
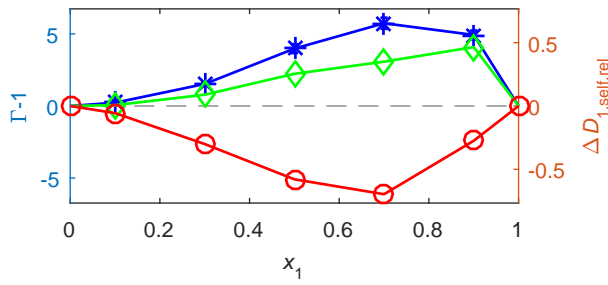
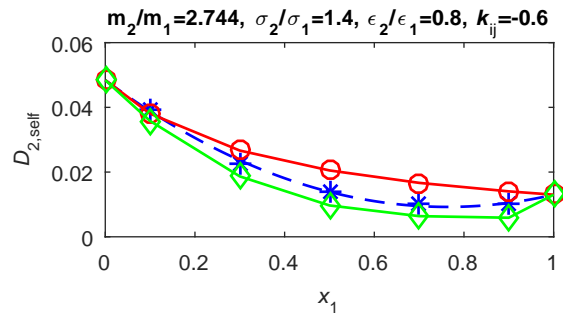
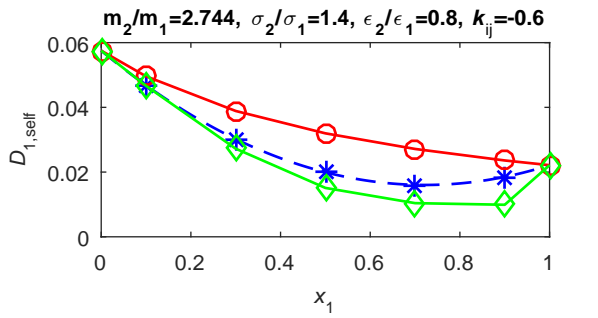
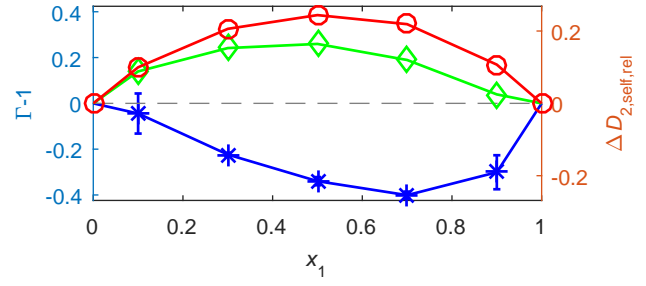
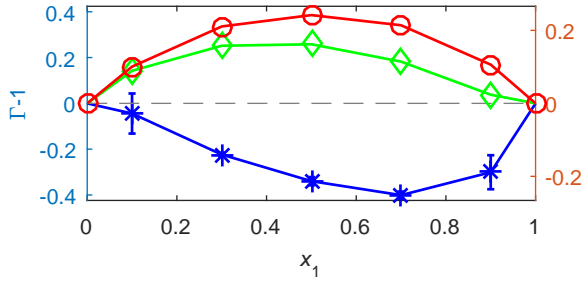
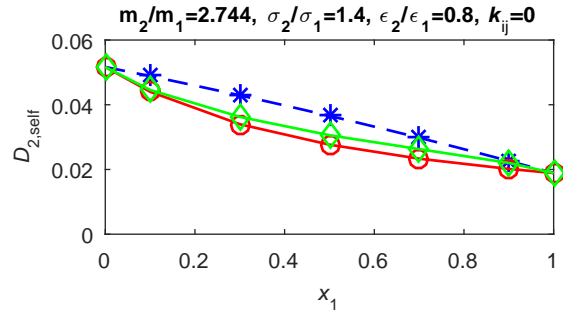
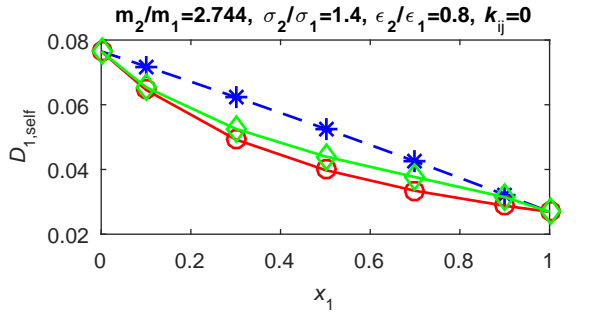
Composition-dependent self-diffusion coefficients $D_{i,\text{self}}$, thermodynamic factors $\Gamma - 1$, and relative deviations $\Delta D_{i,\text{self,rel}}$ of LJ systems with molar mass ratios $m_2/m_1 > 2$. The specifications of the LJ systems ϵ_2/ϵ_1 , σ_2/σ_1 , m_2/m_1 , and k_{ij} are given in the title of each figure.

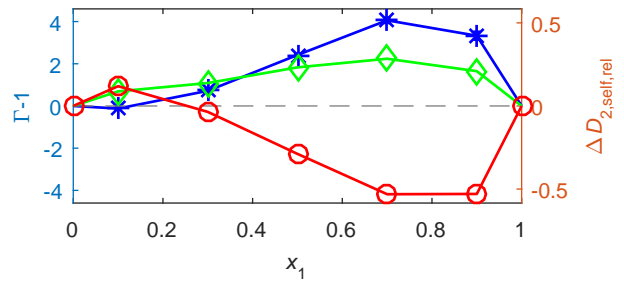
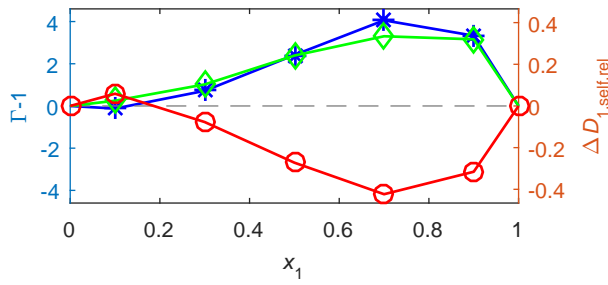
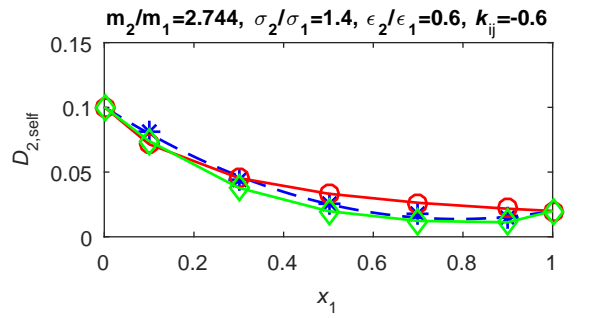
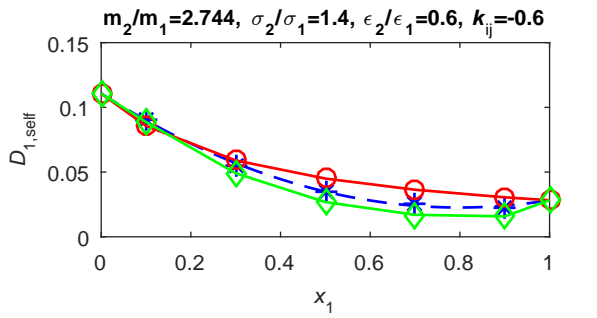
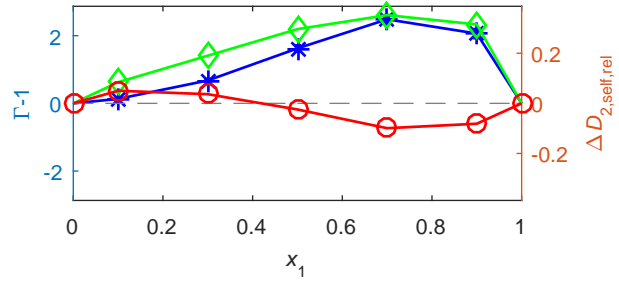
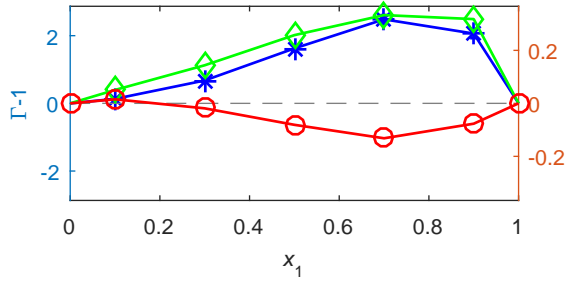
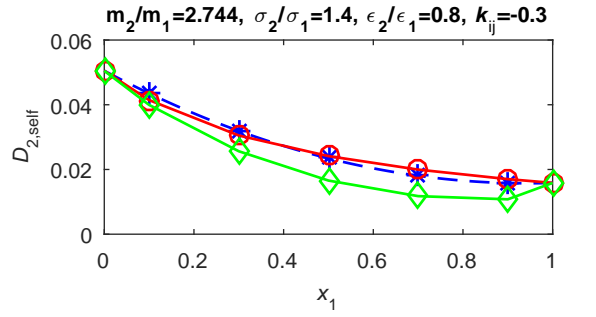
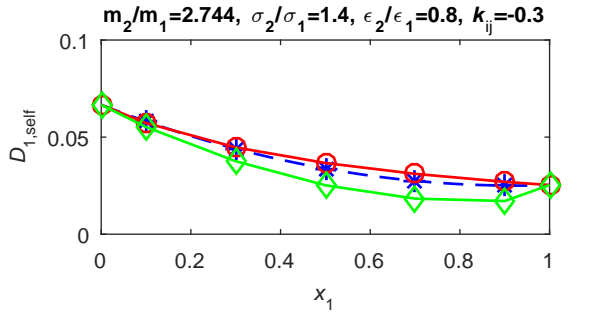
Top figures: Blue stars: Simulation results of self-diffusion coefficients $D_{i,\text{self}}$ of binary LJ systems as function of the mole fraction x_1 of the first species. Blue dashed line: smoothing fit to the simulation results; red circles/line: predictions of the McCarty-Mason equation (Equation 6); green diamonds/line: predictions of the modified McCarty-Mason equation (Equation 25). The error bars of $D_{i,\text{self}}$ are smaller than the symbols in most cases. Please note that y -axes are adapted for each system.

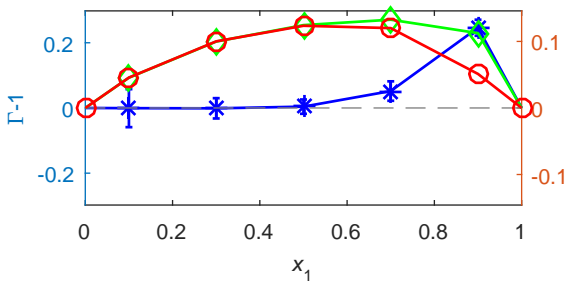
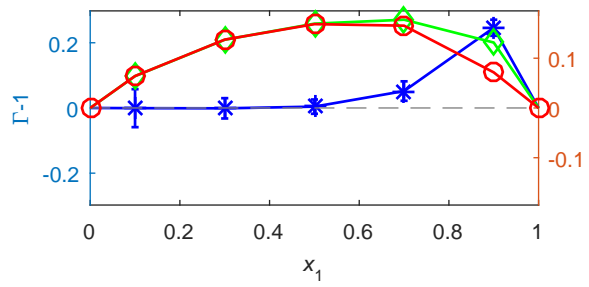
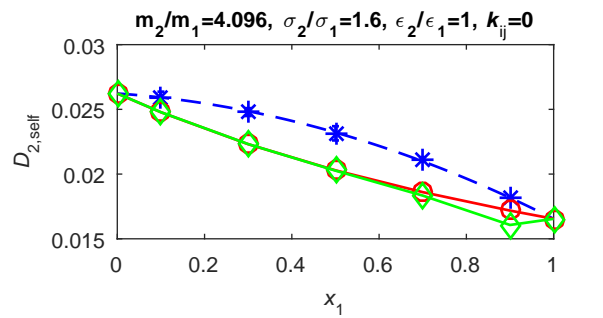
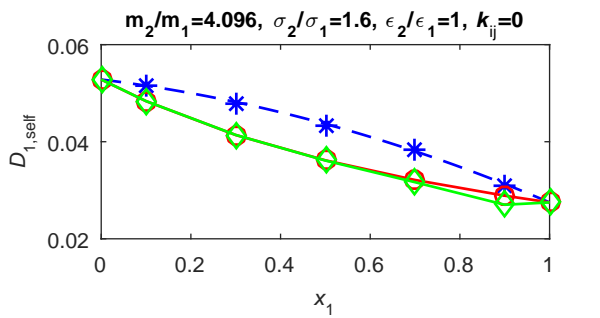
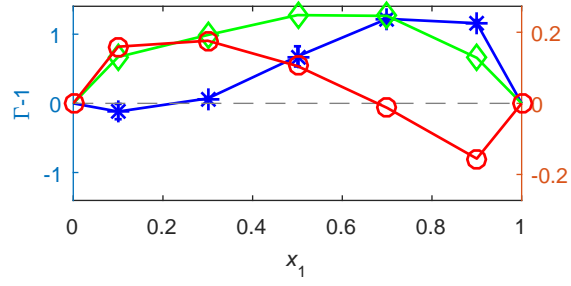
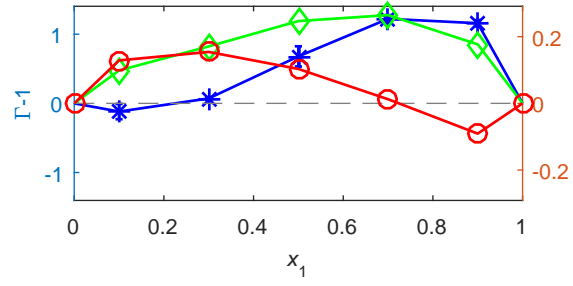
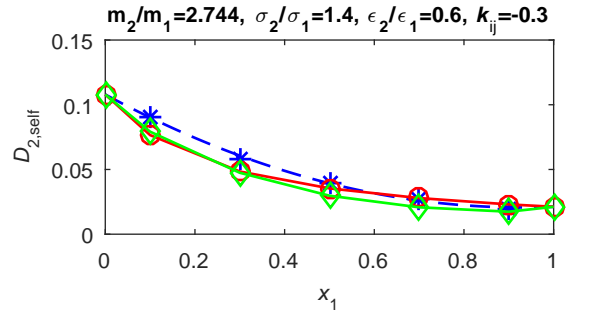
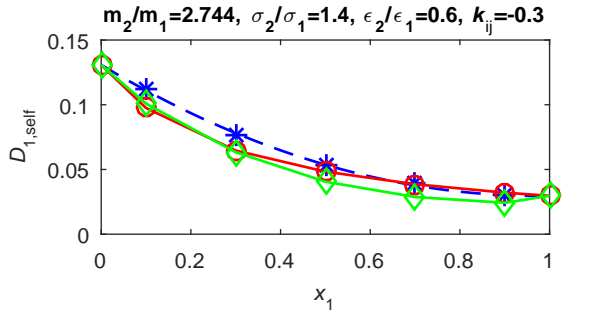
Bottom figures: Composition dependence of the thermodynamic factor $\Gamma - 1$ (blue stars/line, left axis) and composition dependence of the relative deviation $\Delta D_{i,\text{self,rel}}$ between the self-diffusion coefficients and the predictions of the McCarty-Mason equation (Equation 6) (red circles/line, right axis) and the modified McCarthy-Mason equation (Equation 25) (green diamonds/line, right axis). A clear correlation between $\Gamma - 1$ and $\Delta D_{i,\text{self,rel}}$ can be observed. The error bars of $\Gamma - 1$ are smaller than the symbols in most cases. Please note that y -axes are adapted for each system.

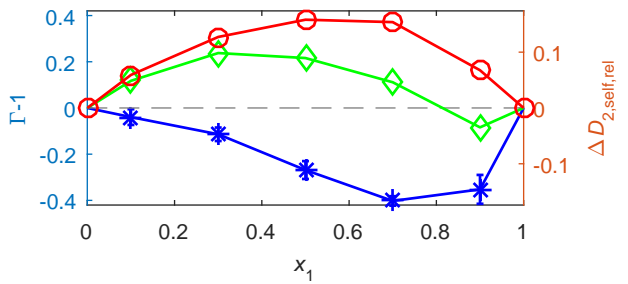
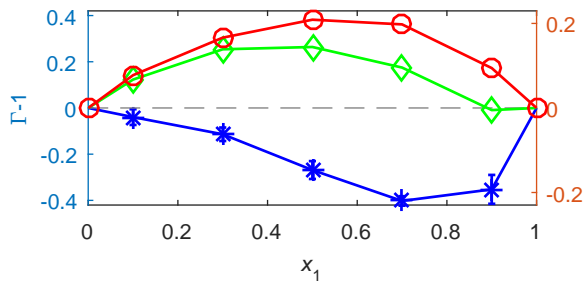
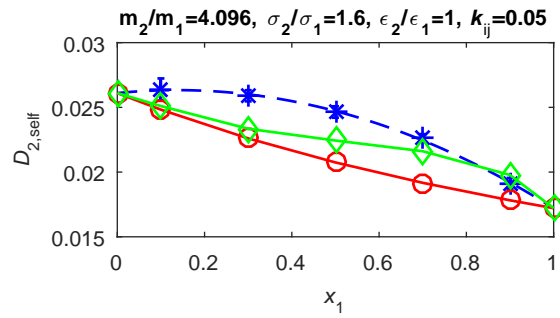
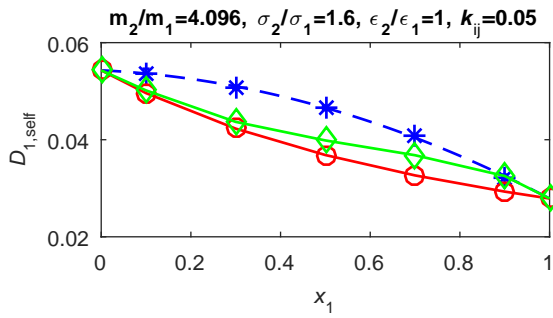
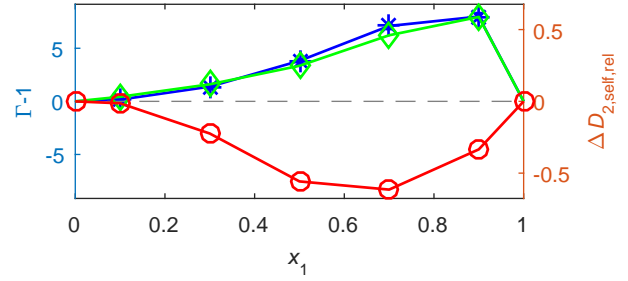
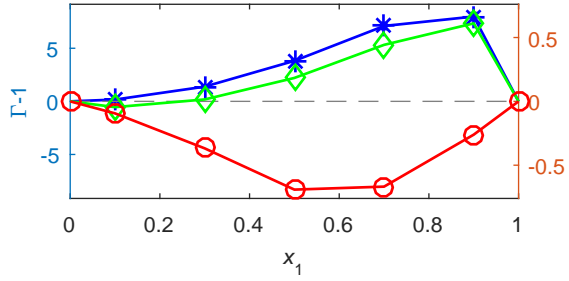
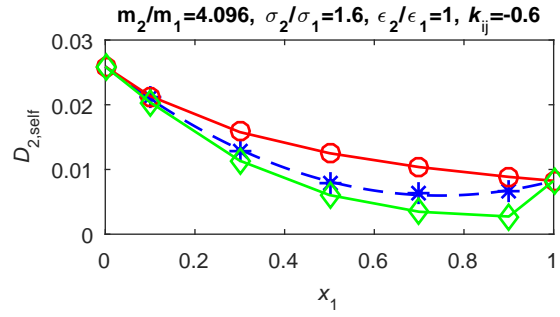
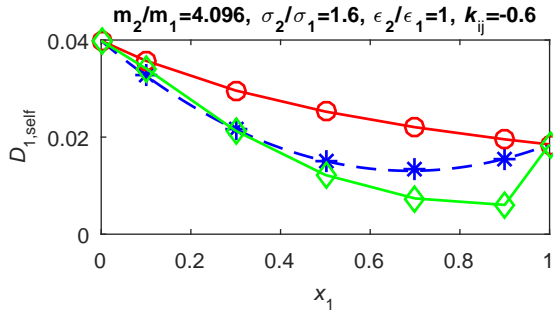


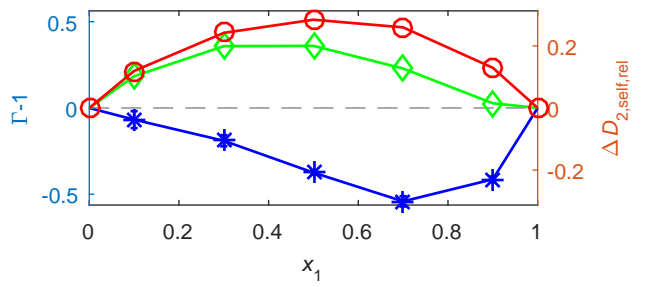
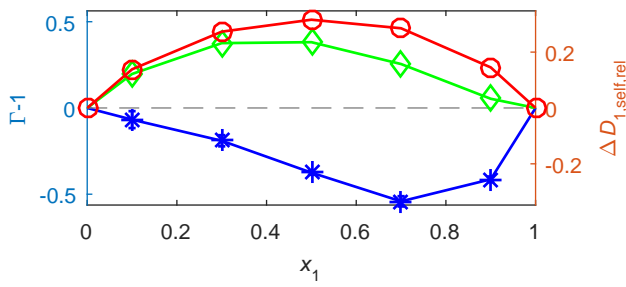
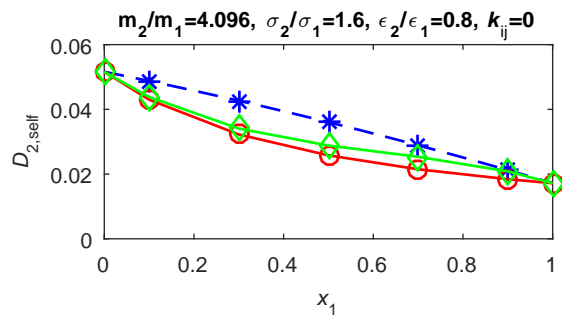
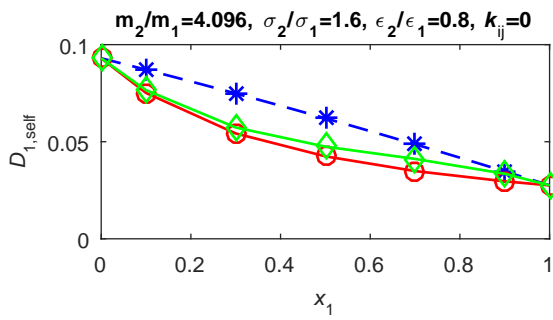
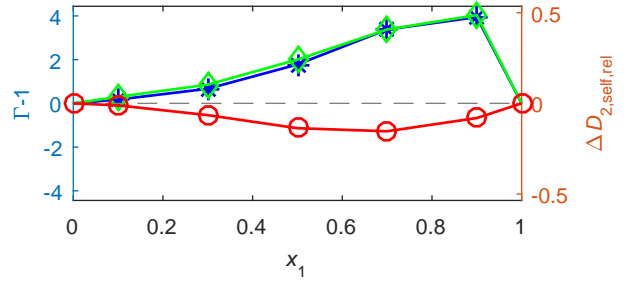
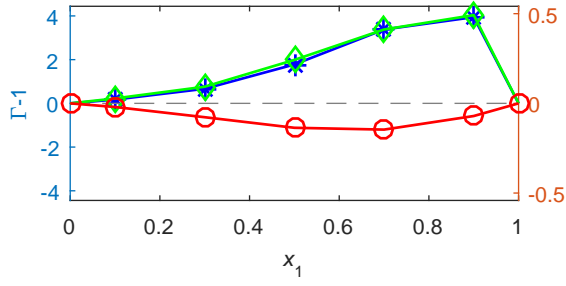
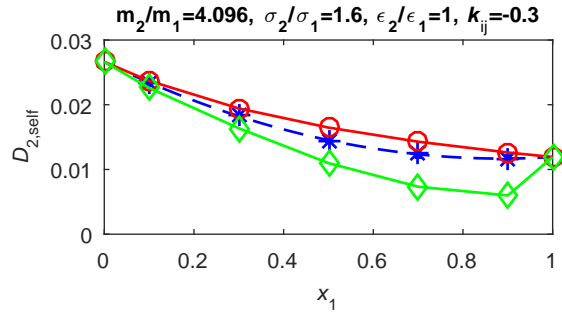
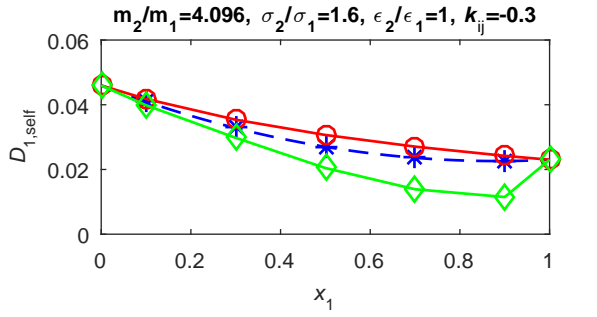


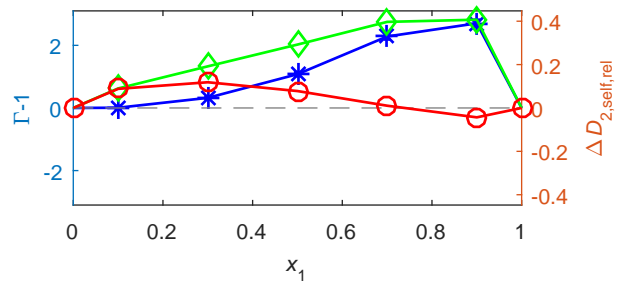
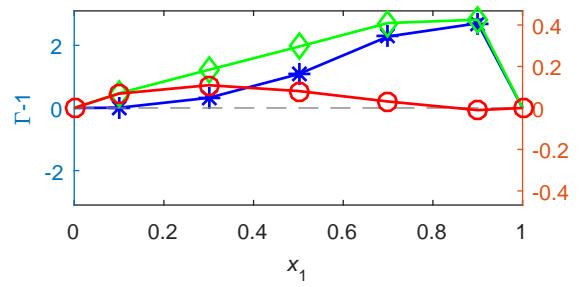
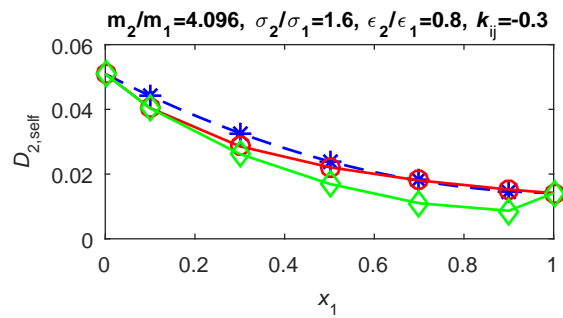
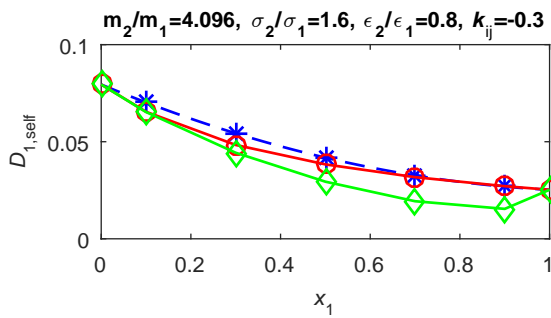
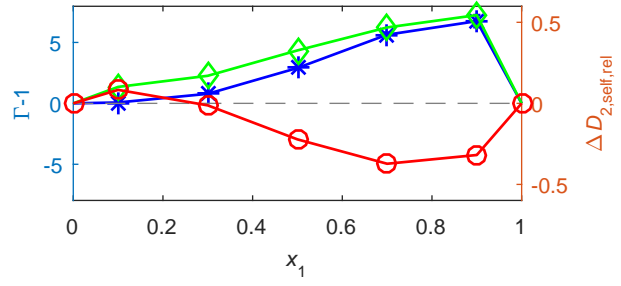
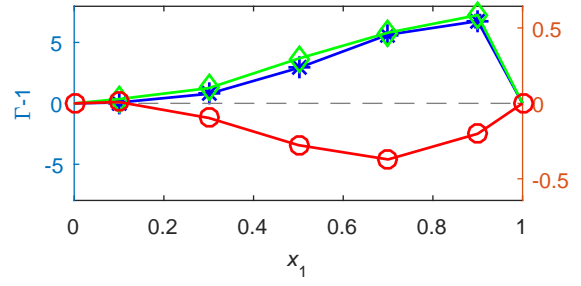
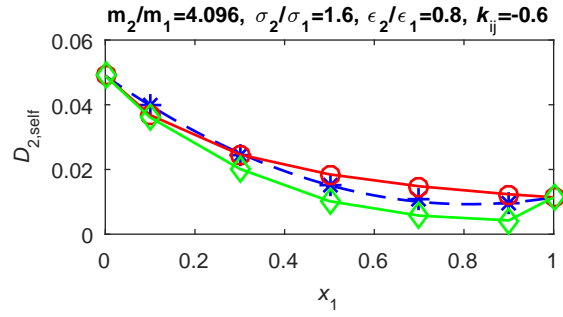
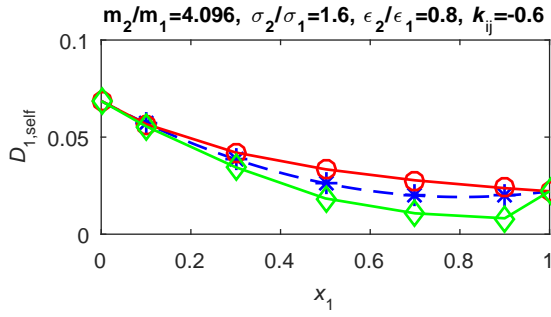


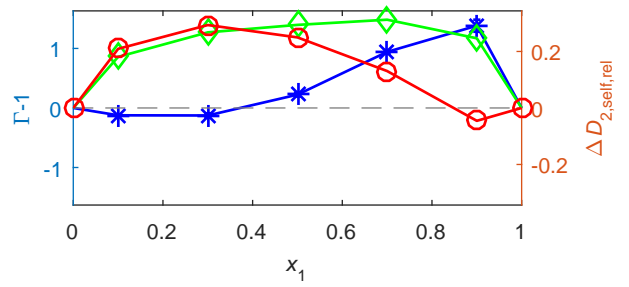
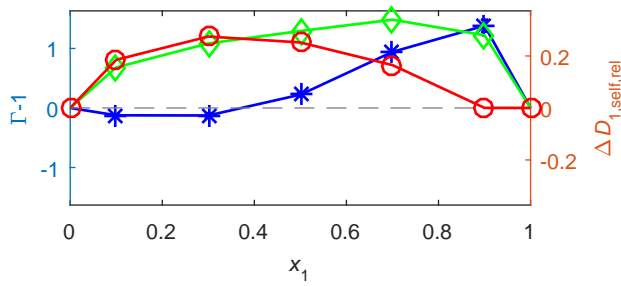
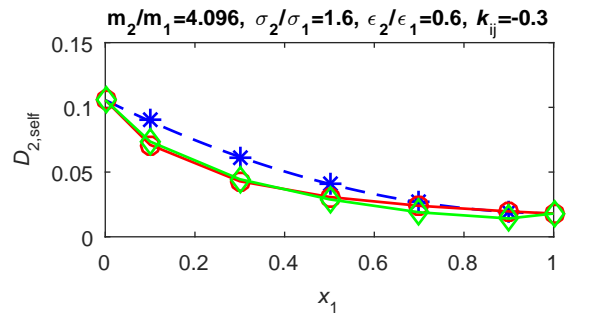
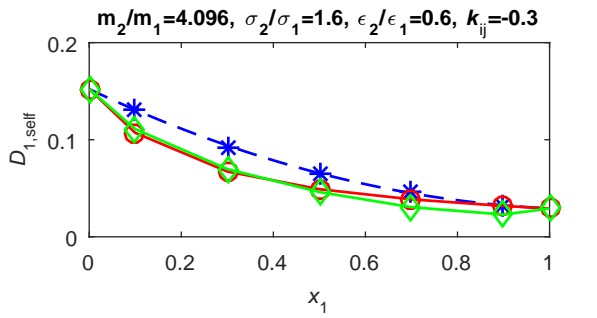
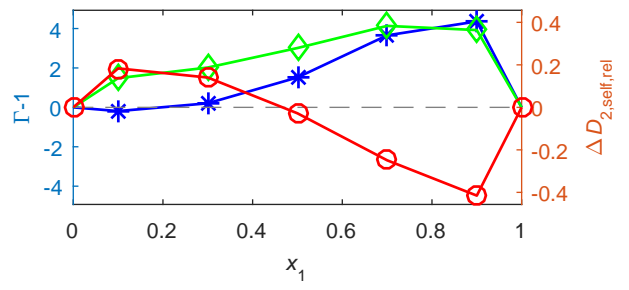
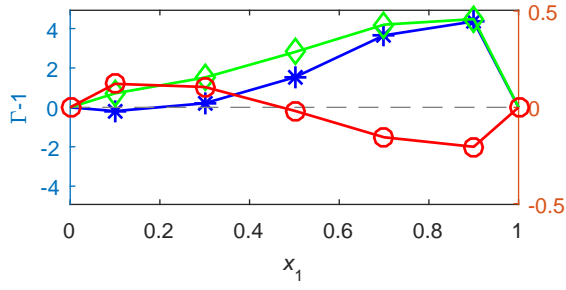
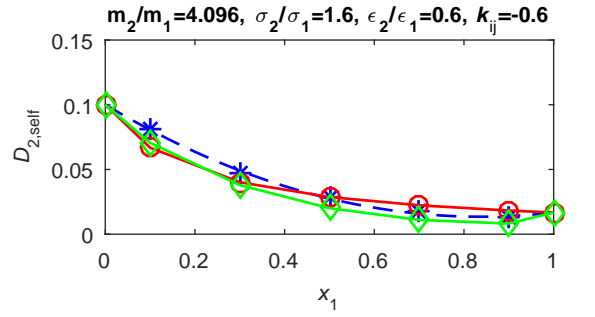
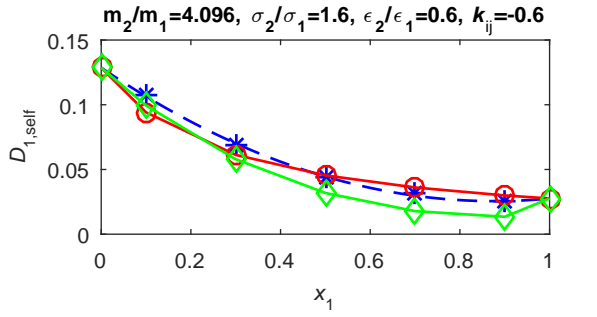


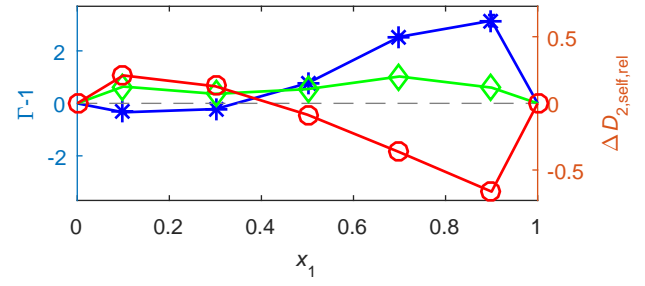
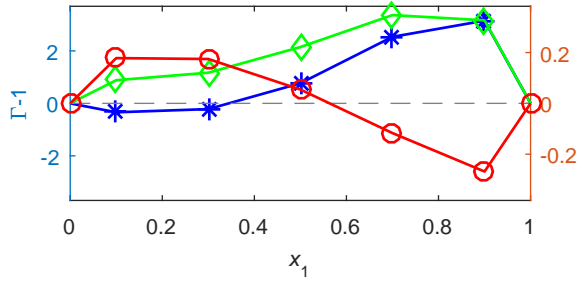
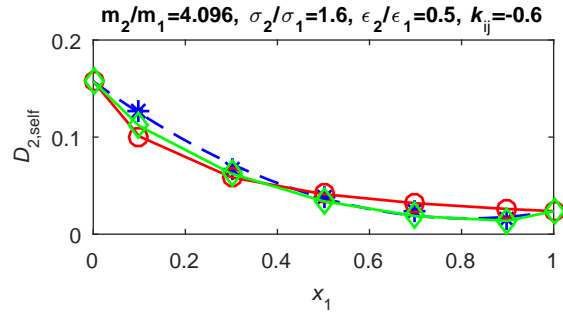
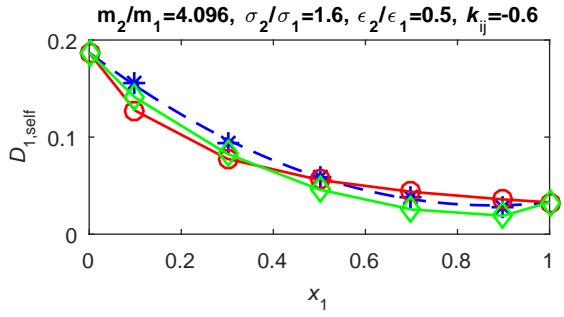












S2 Self-diffusion coefficients of molecular systems (experimental data)

S2.1 Relative deviations $\Delta D_{2,\text{self,rel}}$ of the McCarty-Mason prediction as a function of the thermodynamic factor Γ for component 2

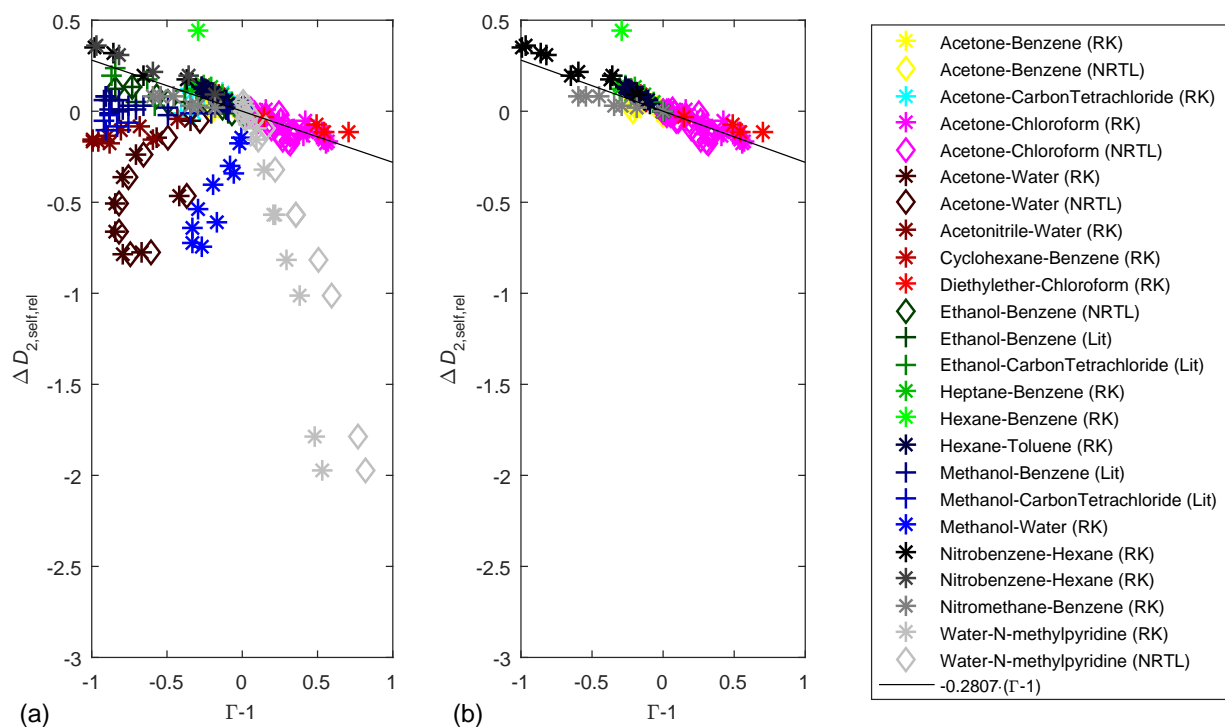


Figure S2: Relative deviations $\Delta D_{2,\text{self,rel}}$ of the McCarty-Mason prediction (Equation (6)) as function of the thermodynamic factor Γ for molecular systems (symbols) and linear fit of $\Delta D_{2,\text{self,rel}}$ derived from LJ systems (black line, cf. Equation (23)). Stars: Experimental data with thermodynamic factors calculated with Redlich-Kister (RK). Diamonds: Experimental data with thermodynamic factors calculated with NRTL. Plus symbols: Experimental data with thermodynamic factors reported in literature.

(a) $\Delta D_{2,\text{self,rel}}$ for all considered molecular systems.

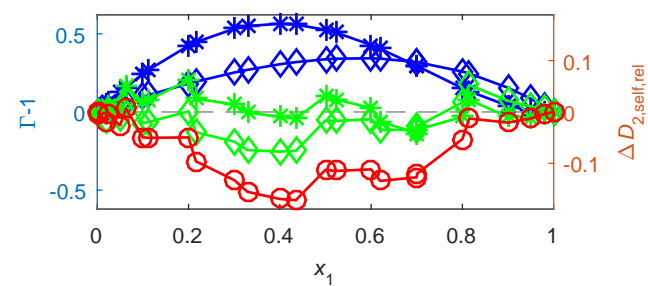
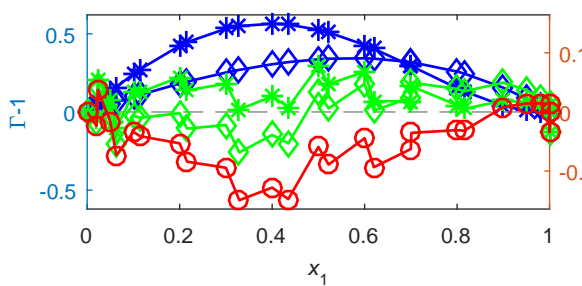
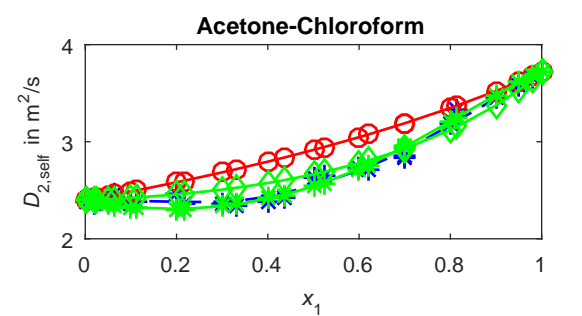
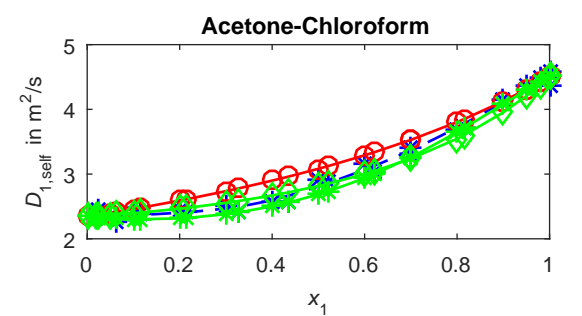
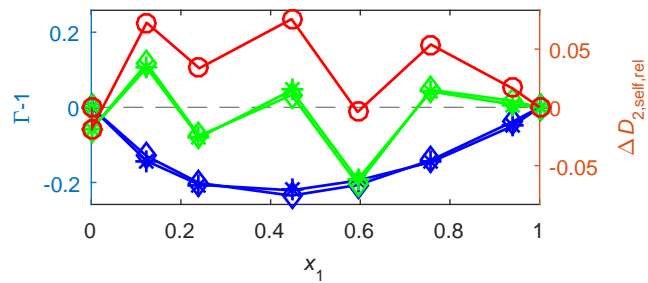
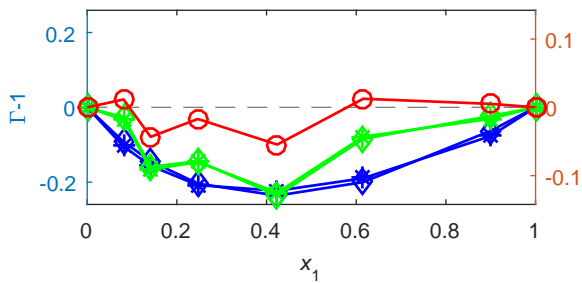
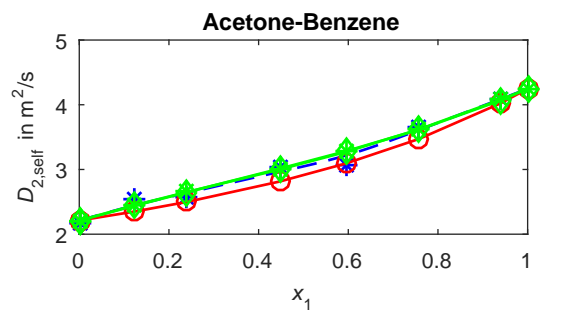
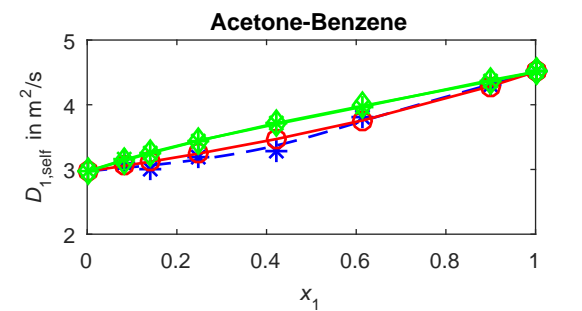
(b) $\Delta D_{2,\text{self,rel}}$ for molecular systems with molar mass ratios $M_2/M_1 < 2$ and without dimerising species.

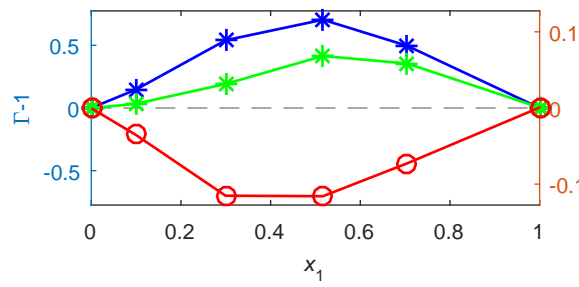
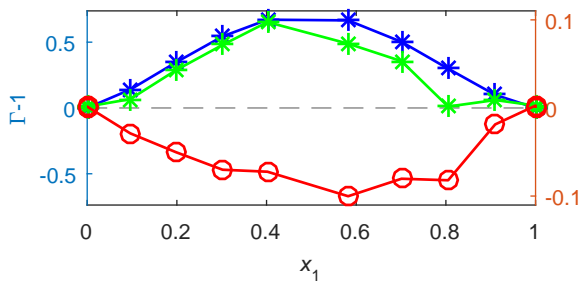
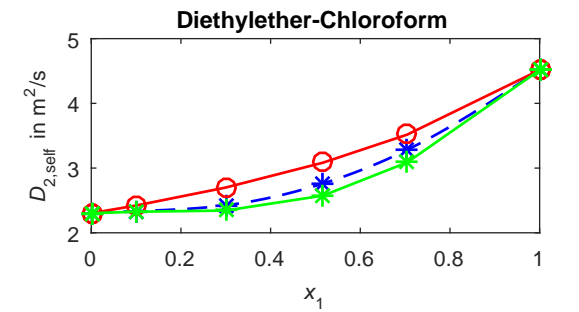
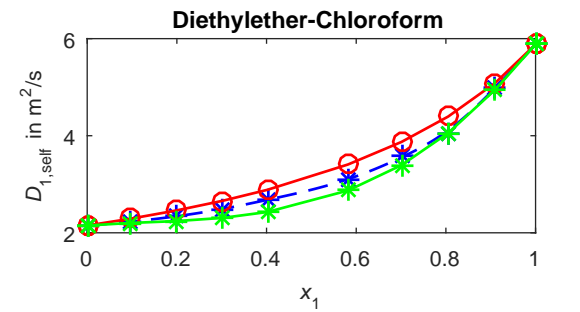
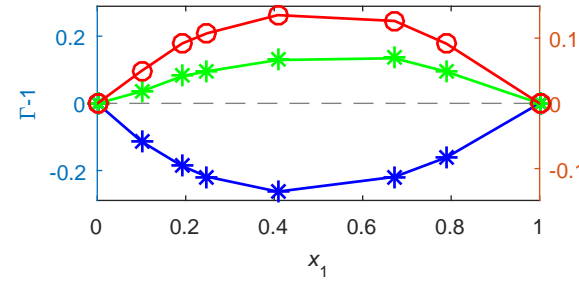
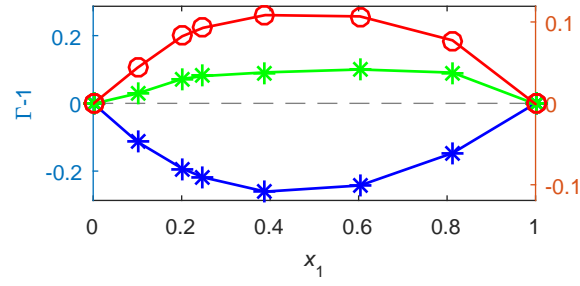
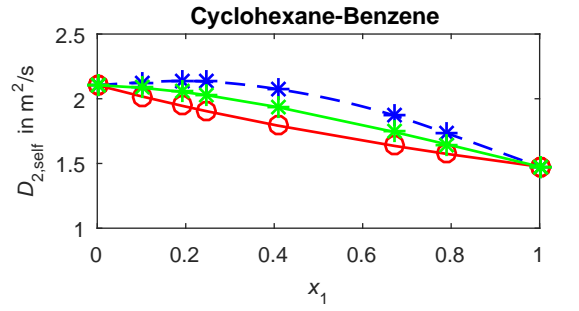
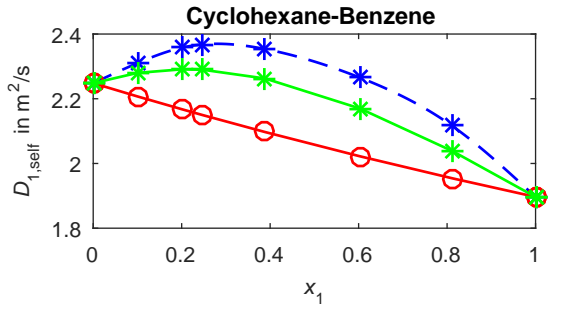
S2.2 Molecular systems with molar mass ratios $M_2/M_1 < 2$ and without dimerising species

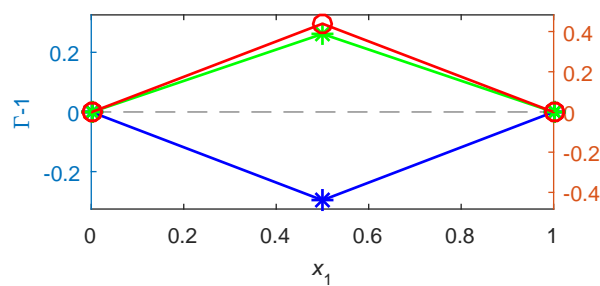
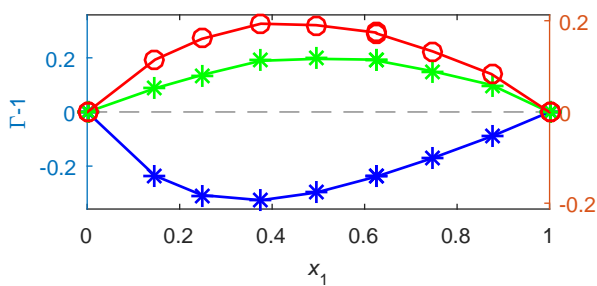
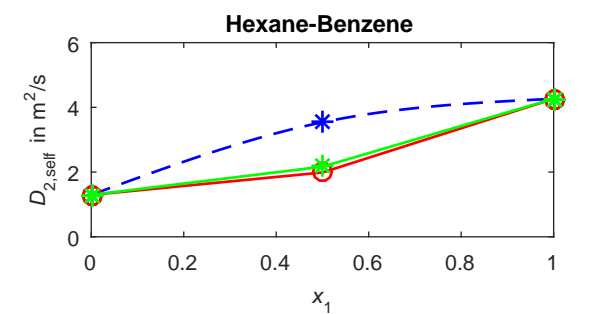
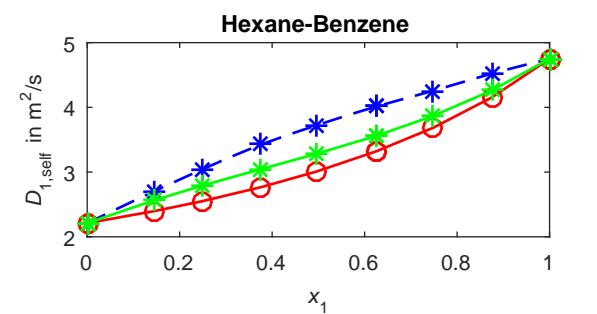
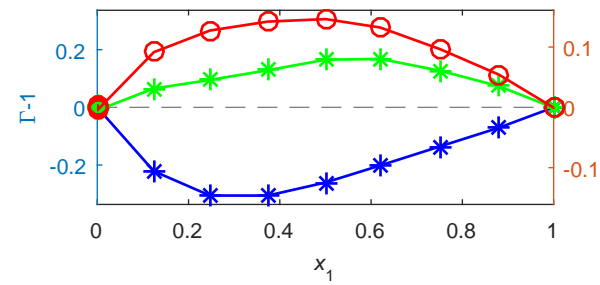
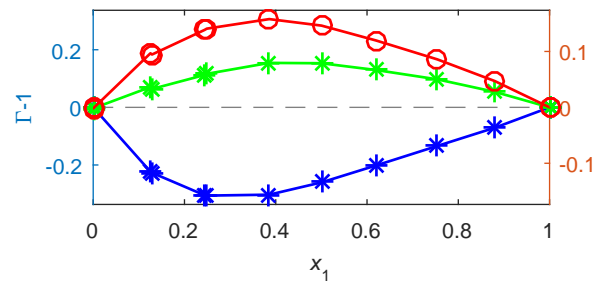
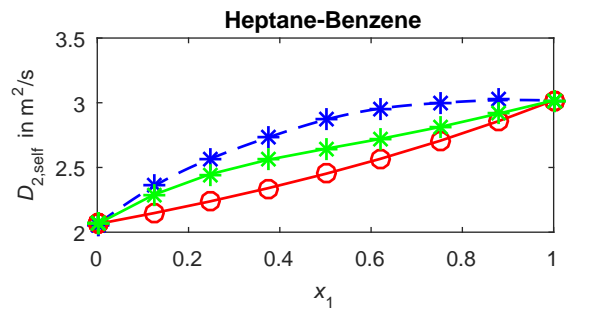
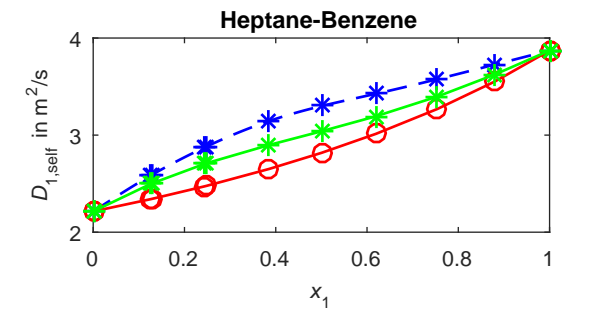
Composition-dependent self-diffusion coefficients $D_{i,\text{self}}$, thermodynamic factors $\Gamma - 1$, and relative deviations $\Delta D_{i,\text{self,rel}}$ of molecular systems with molar mass ratios $M_2/M_1 < 2$ and without dimerising species. The specific components of each molecular system are given in the title of each figure.

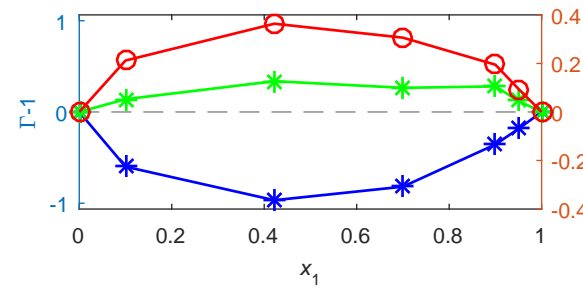
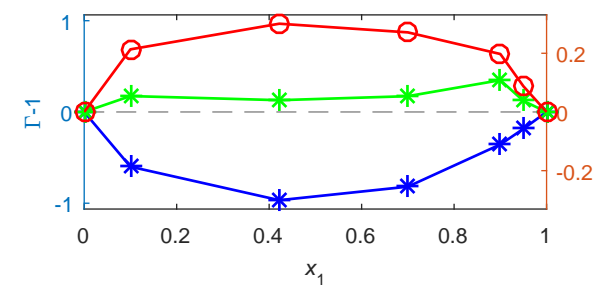
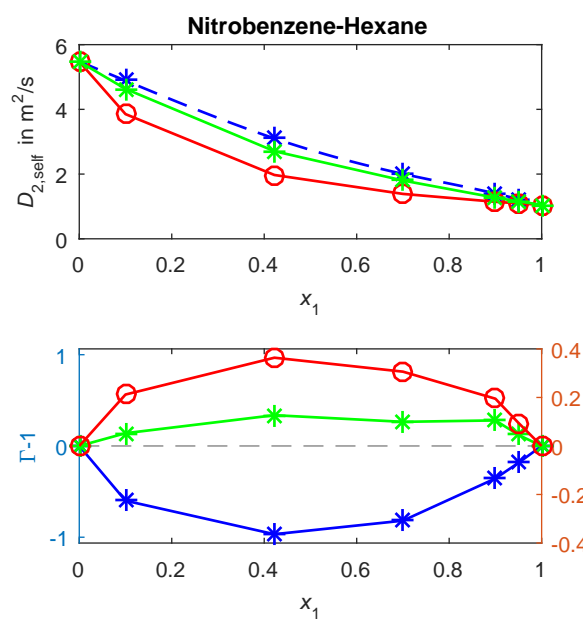
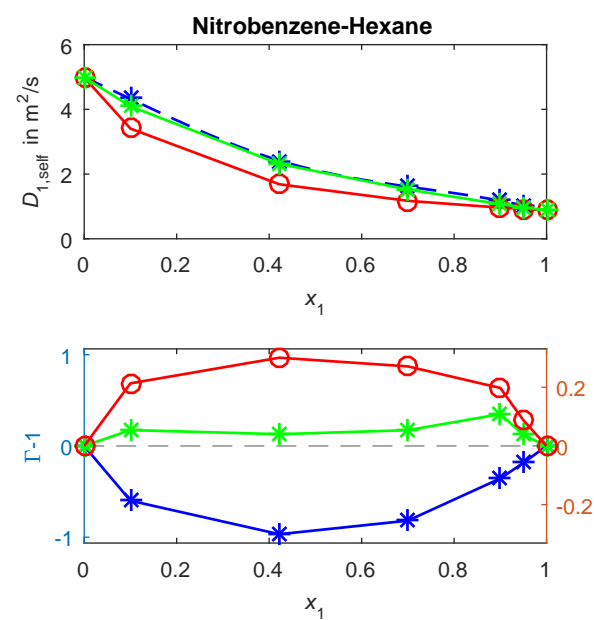
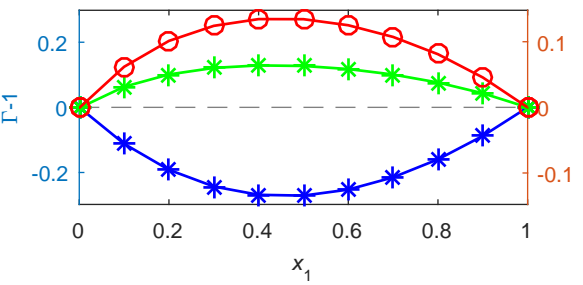
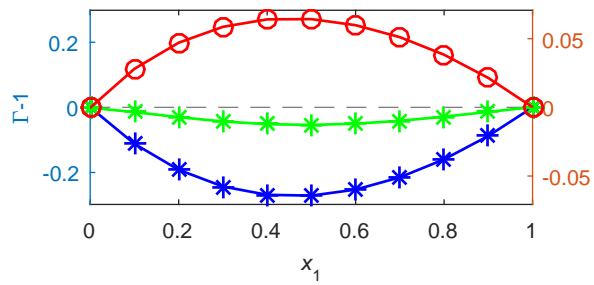
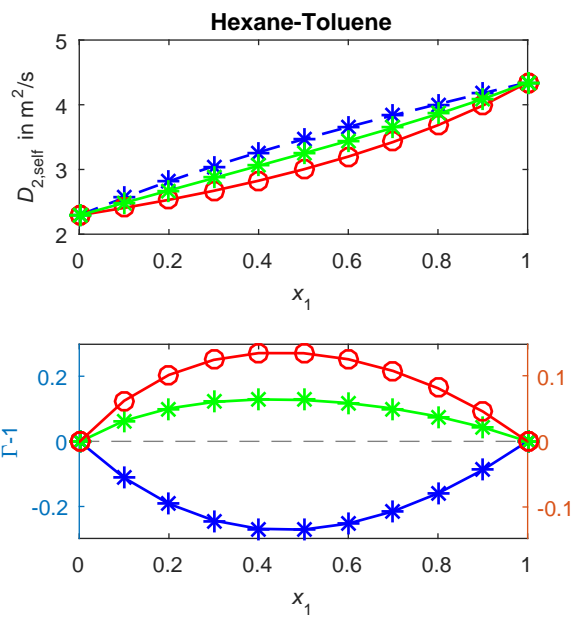
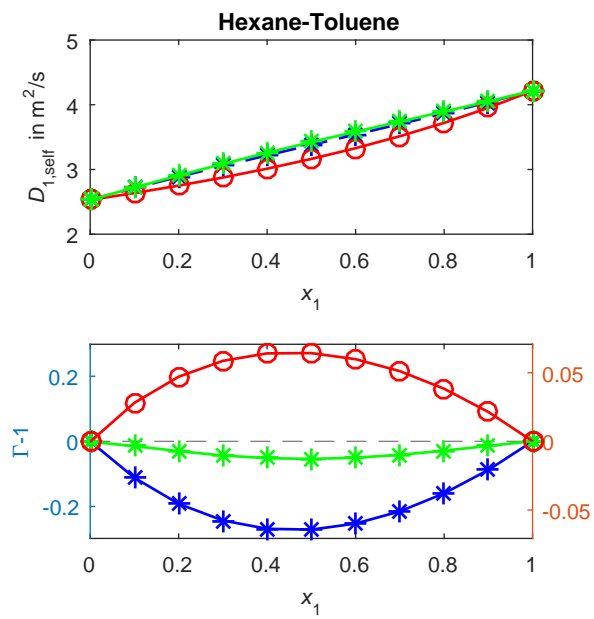
Top figures: Blue stars: Experimental data of composition-dependent self-diffusion coefficients $D_{i,\text{self}}$. Blue dashed line: smoothing fit of the experimental self-diffusion coefficients; red circles/line: predictions of the McCarty-Mason equation (Equation 6); green diamonds/line: predictions of the modified McCarty-Mason equation (Equation 25).

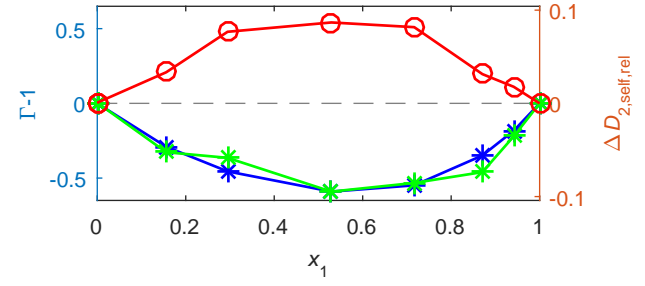
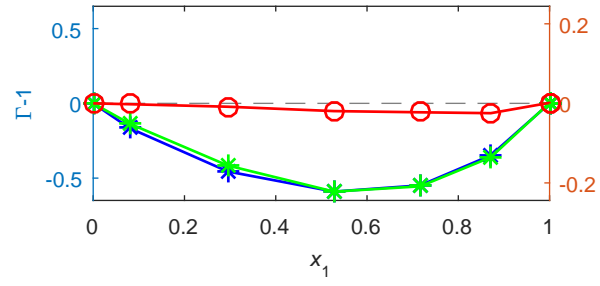
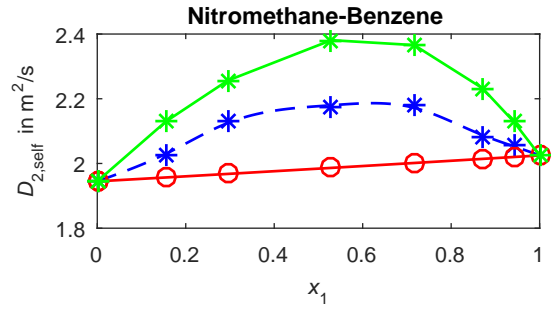
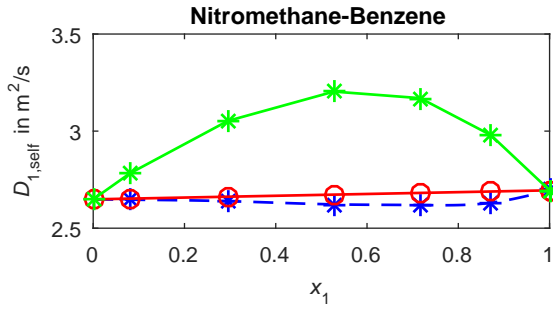
Bottom figures: Composition dependence of the thermodynamic factor $\Gamma - 1$ (blue symbols/line, left axis) and composition dependence of the relative deviation $\Delta D_{i,\text{self,rel}}$ between the experimental self-diffusion coefficients and the predictions of the McCarty-Mason equation (Equation 6) (red circles/line, right axis) and the modified McCarthy-Mason equation (Equation 25) (green symbols/line, right axis). The symbols for the thermodynamic factors and the predictions of the modified McCarty-Mason predictions indicate the source of the thermodynamic factor calculations: Redlich-Kister (stars), NRTL (diamonds), or reported directly in literature (crosses).









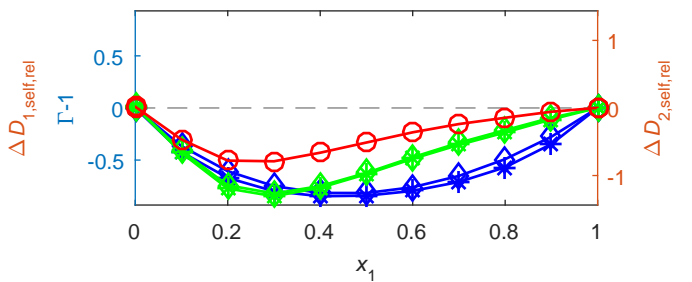
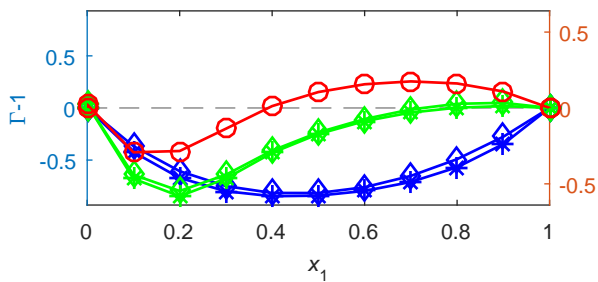
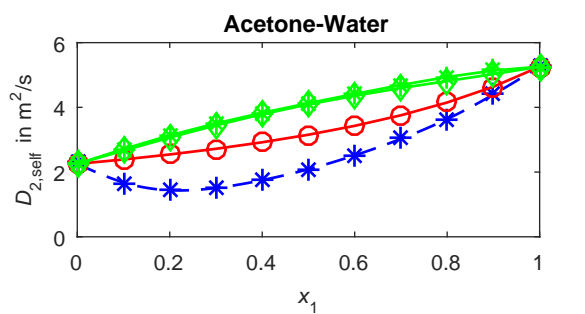
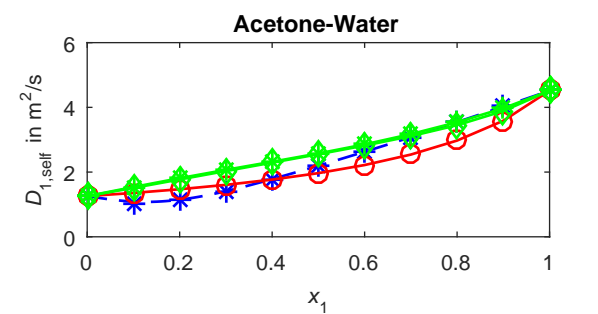
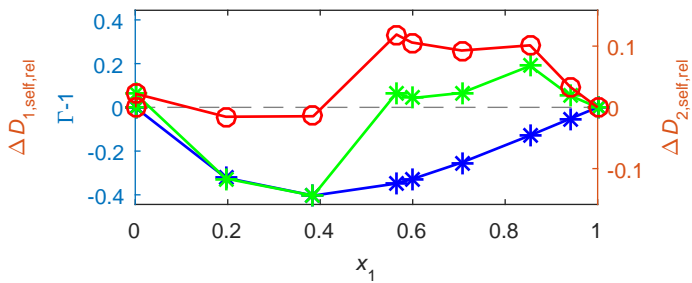
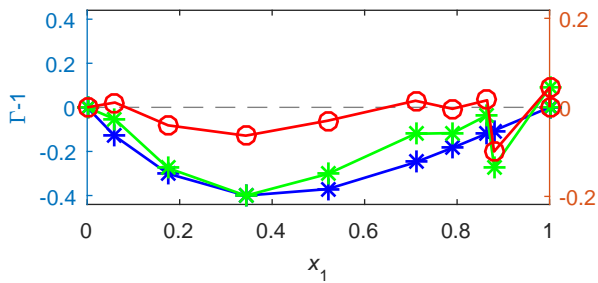
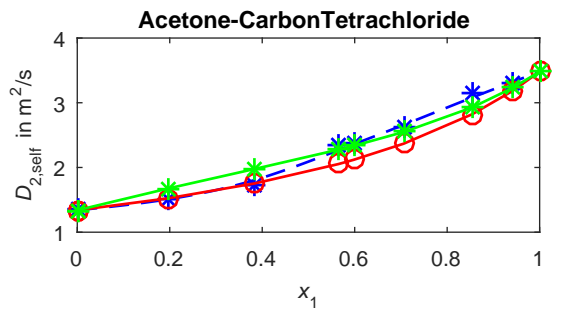
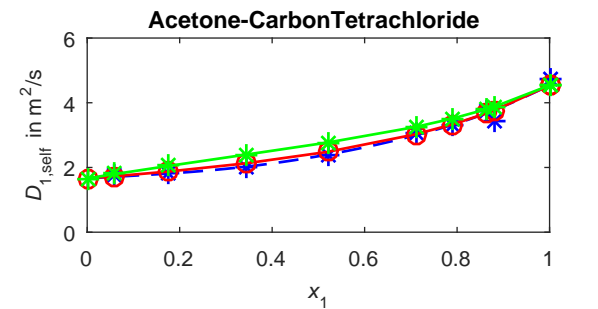


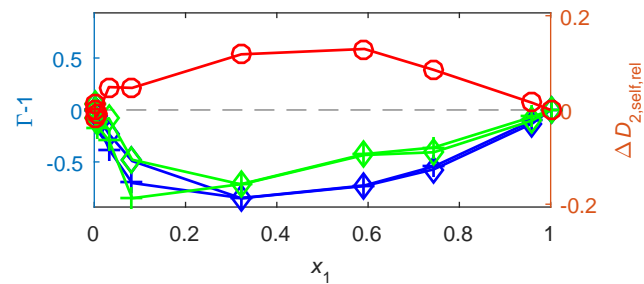
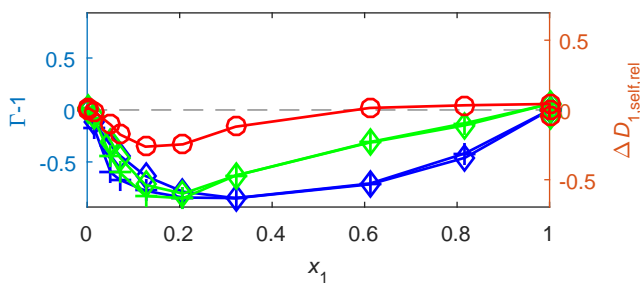
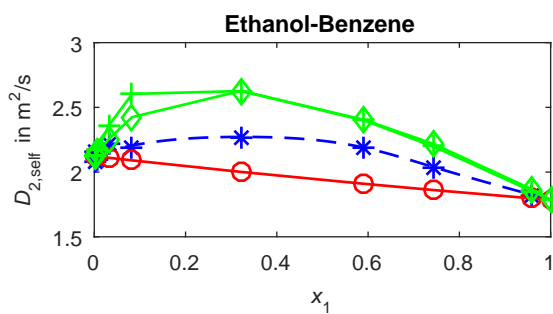
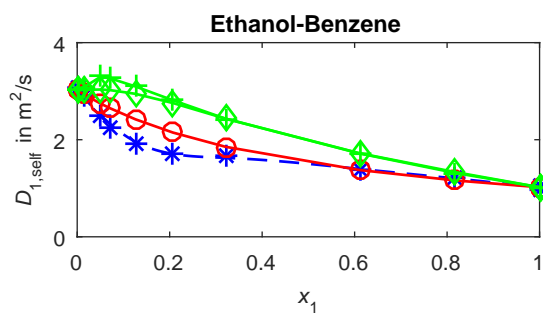
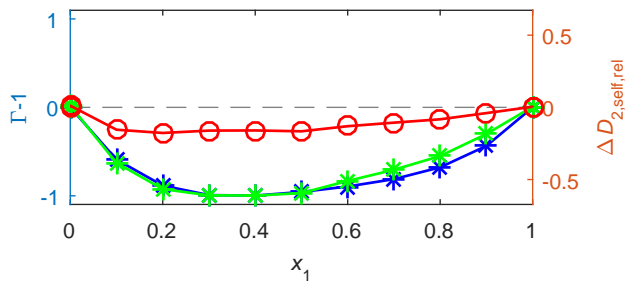
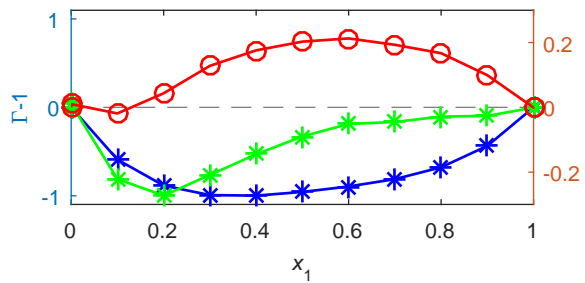
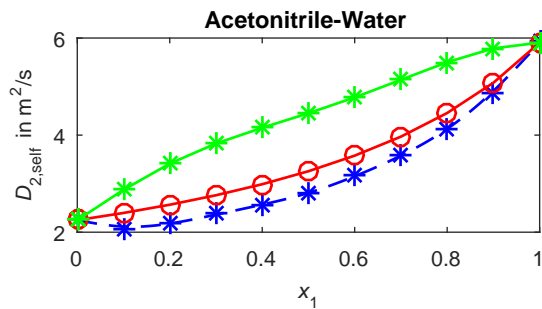
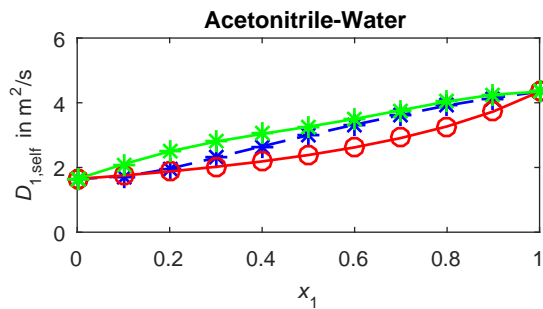
S2.3 Molecular systems with molar mass ratios $M_2/M_1 > 2$ and/or with dimerising species

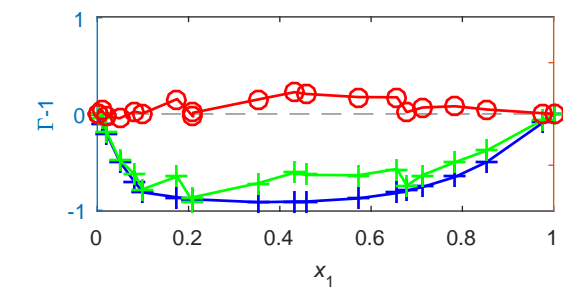
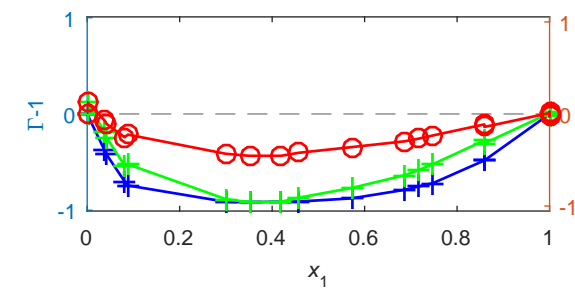
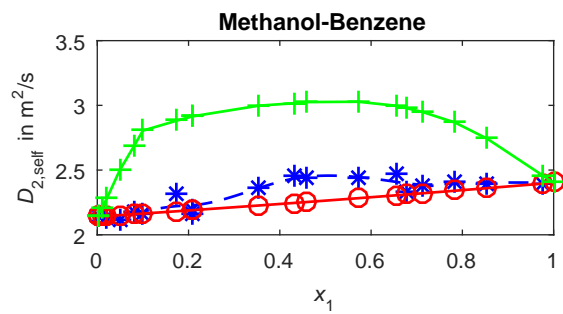
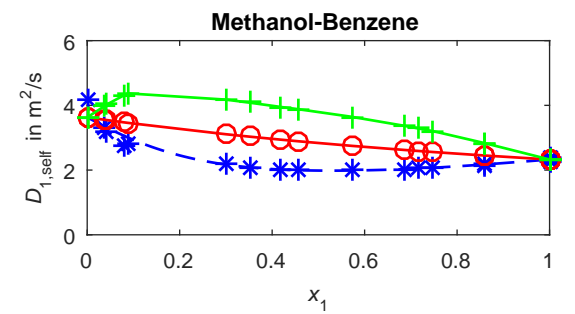
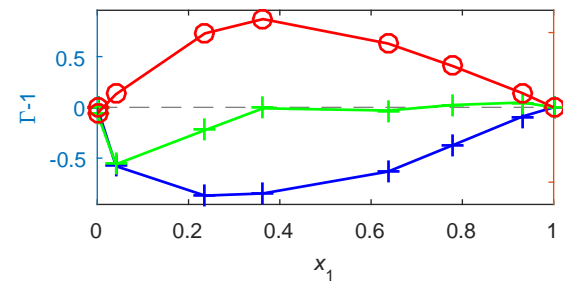
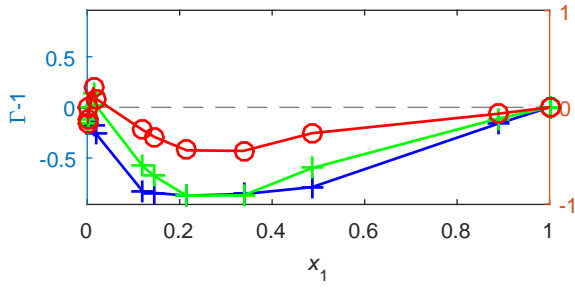
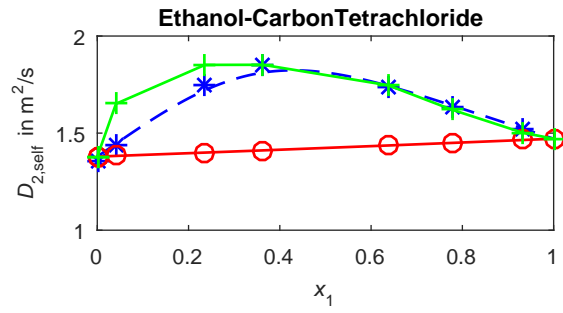
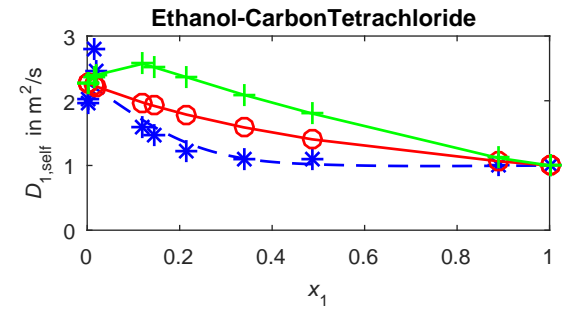
Composition-dependent self-diffusion coefficients $D_{i,\text{self}}$, thermodynamic factors $\Gamma - 1$, and relative deviations $\Delta D_{i,\text{self,rel}}$ of molecular systems with molar mass ratios $M_2/M_1 > 2$ and/or with dimerising species. The specific components of each molecular system are given in the title of each figure.

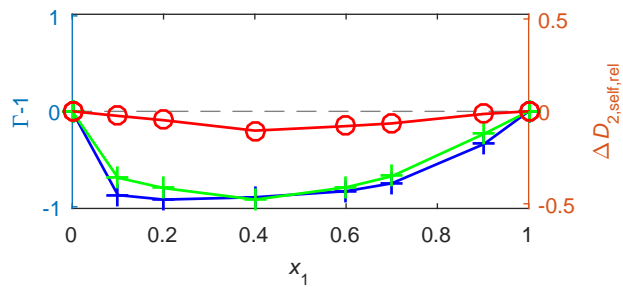
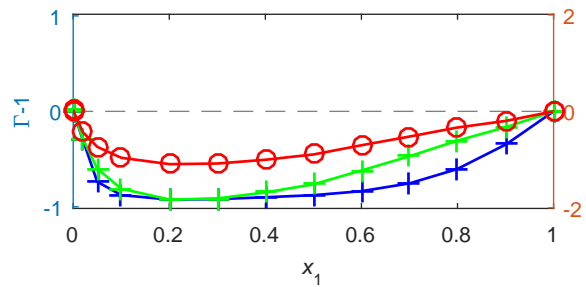
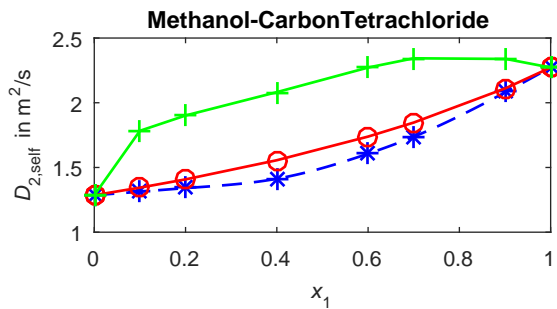
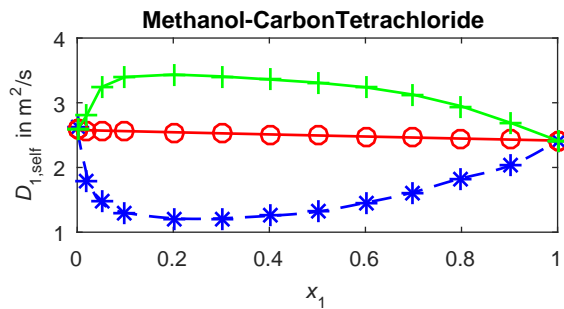
Top figures: Blue stars: Experimental data of composition-dependent self-diffusion coefficients $D_{i,\text{self}}$. Blue dashed line: smoothing fit of the experimental self-diffusion coefficients; red circles/line: predictions of the McCarty-Mason equation (Equation 6); green diamonds/line: predictions of the modified McCarty-Mason equation (Equation 25).

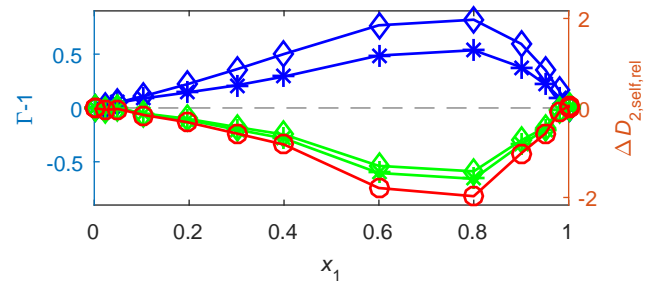
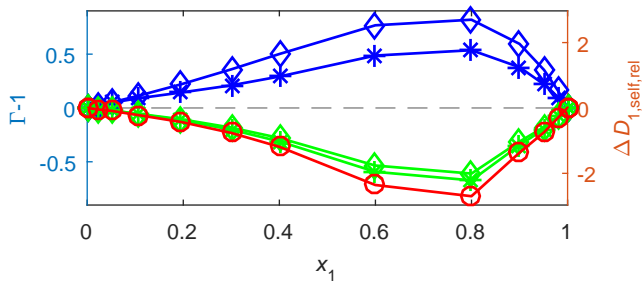
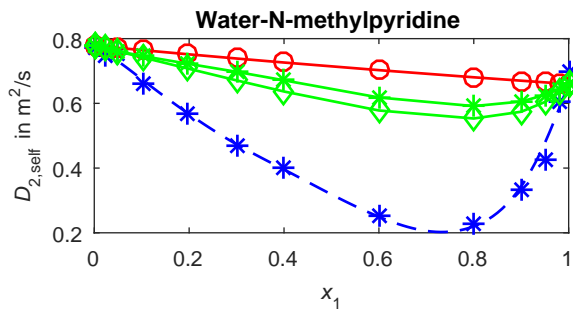
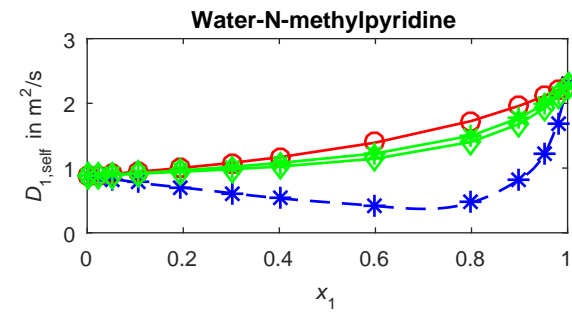
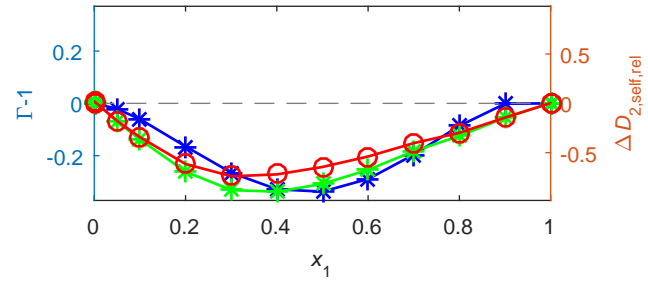
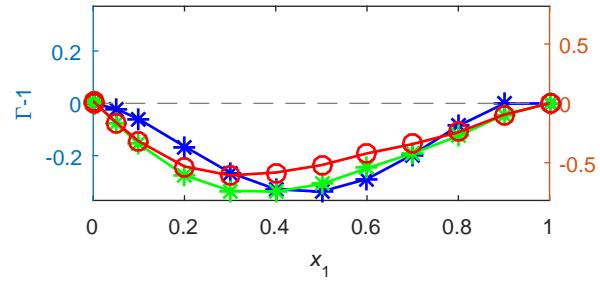
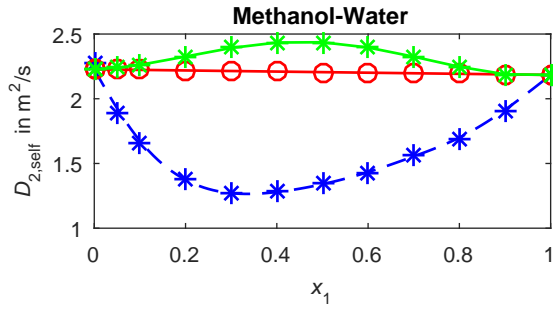
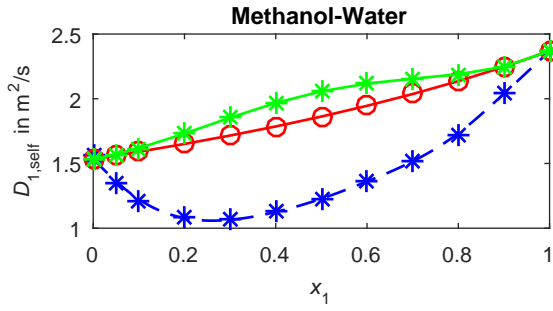
Bottom figures: Composition dependence of the thermodynamic factor $\Gamma - 1$ (blue symbols/line, left axis) and composition dependence of the relative deviation $\Delta D_{i,\text{self,rel}}$ between the experimental self-diffusion coefficients and the predictions of the McCarty-Mason equation (Equation 6) (red circles/line, right axis) and the modified McCarty-Mason equation (Equation 25) (green symbols/line, right axis). The symbols for the thermodynamic factors and the predictions of the modified McCarty-Mason predictions indicate the source of the thermodynamic factor calculations: Redlich-Kister (stars), NRTL (diamonds), or reported directly in literature (crosses).











S3 References for the experimental data used in this work

Table S1: References for the experimental data used in this work.

System	Diffusion coefficients			Thermodynamic factor		
	D_{12}	$D_{1,self}$	$D_{2,self}$	Redlich-Kister (RK)	NRTL	reported in Literature (Lit)
Acetone-Benzene	Anderson et al. ¹ , Cullinan and Toor ⁵	Yoshinobu and Yasumichi ²	Yoshinobu and Yasumichi ²	Moggridge ³	Zhu et al. ⁴	-
Acetone-CarbonTetrachloride	Anderson et al. ¹ , Cullinan and Toor ⁵	Hardt et al. ⁶	Hardt et al. ⁶	Moggridge ³	-	-
Acetone-Chloroform	McCall and Douglass ⁷ , Tyn and Calus ¹⁰ , Anderson et al. ¹	D'Agostino et al. ⁸	D'Agostino et al. ⁸	D'Agostino et al. ⁸	Gmehling et al. ⁹	-
Acetone-Water	Anderson et al. ¹ , Grossmann and Winkelmann ¹² , Rehfeldt and Stichlmair ¹³ , Tyn and Calus ¹⁰ , Zhou et al. ¹⁴	Mills and Hertz ¹¹	Mills and Hertz ¹¹	Moggridge ³	Gmehling et al. ⁹	-
Acetonitrile-Water	Easteal et al. ¹⁵	Easteal et al. ¹⁵	Easteal et al. ¹⁵	Fitted from data of French ¹⁶	-	-
Cyclohexane-Benzene	Harned ¹⁷	Mills ¹⁸	Mills ¹⁸	Moggridge ³	-	-
Diethylether-Chloroform	Sanni et al. ¹⁹ , Weingärtner ²⁰	Weingärtner ²⁰	Weingärtner ²⁰	Moggridge ³	-	-
Ethanol-Benzene	Anderson et al. ¹ , Zhu et al. ⁴	Johnson and Babb ²¹	Johnson and Babb ²¹	-	Zhu et al. ⁴	Guevara-Carrion et al. ^{22*}
Ethanol-Carbon Tetrachloride	Hammond and Stokes ²³ , Longsworth ²⁴ , Bosse and Bart ²⁵	Hardt et al. ⁶	Hardt et al. ⁶	-	-	Guevara-Carrion et al. ^{22*}
Heptane-Benzene	Harris et al. ²⁶	Harris et al. ²⁶	Harris et al. ²⁶	Moggridge ³	-	-
Hexane-Benzene	Harris et al. ²⁶	Harris et al. ²⁶	Harris et al. ²⁶	Moggridge ³	-	-
Hexane-Toluene	Ghai and Dullien ²⁷	Ghai and Dullien ²⁷	Ghai and Dullien ²⁷	Moggridge ³	-	-
Methanol-Benzene	Caldwell and Babb ²⁸	Aoyagi and Albright ²⁹ , Johnson and Babb ²¹	Aoyagi and Albright ²⁹ , Johnson and Babb ²¹	-	-	Guevara-Carrion et al. ^{22*}
Methanol-Carbon Tetrachloride	Anderson et al. ¹ , Prabhakar and Weingärtner ³⁰ , Longsworth ²⁴	Prabhakar and Weingärtner ³⁰	Prabhakar and Weingärtner ³⁰	-	-	Guevara-Carrion et al. ^{22*}
Methanol-Water	Chang et al. ³¹ , Derlacki et al. ³² , Bosse and Bart ²⁵	Derlacki et al. ³²	Derlacki et al. ³²	Moggridge ³	-	-
Nitrobenzene-Hexane	Haase and Siry ³³	D'Agostino et al. ³⁴	D'Agostino et al. ³⁴	D'Agostino et al. ³⁴	-	-
Water-N-methylpyridine	Ambrosone et al. ³⁵	Ambrosone et al. ³⁵	Ambrosone et al. ³⁵	Moggridge ³	Zhu et al. ⁴	-

*MD simulation results verified with experimental data

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