

Supplementary Material

Automation of diffusion database development in multicomponent alloys from large number of experimental composition profiles

Jing Zhong¹, Li Chen¹, Lijun Zhang^{1,2,*}

¹State Key Laboratory of Powder Metallurgy, Central South University, Changsha, Hunan 410083, China

²Shenzhen Research Institute, Central South University, Shenzhen 518057, China

*Corresponding author. E-mail: lijun.zhang@csu.edu.cn

Supplementary Methods

Preprocessing and data-cleaning: The fitting kernels are developed to deal with three different types of composition profiles, i.e., composition profiles without uphill trending, composition profiles with uphill trending and equal endmembers, as well as composition profiles with uphill trending and unequal endmembers. For the composition profiles without uphill trending, the composition profiles are fitted with the superposition of preset functions, i.e., the logistic function, while the degree of superposition is selected with AIC. For composition profiles with uphill trending and equal endmembers, the superposition of preset functions, i.e., the probability function of various statistic distributions, can be employed, while selection for the most appropriate one is chosen with AIC. For the ones with uphill trending and unequal endmembers, the mixtures of the superposition of the previous two types of the preset functions are capable of the fitting processes.

Convergence diagnosis of the MCMC sequences: To avoid the excessive evaluation, the convergence diagnostic is therefore essential to perceive the state of MCMC results ensuring the satisfactory representative towards the posterior distribution¹¹. Currently, it is assumed that m independent chains and N samples are considered. The between-sequence variance $\mathbf{B}/N$ and the within-sequence variance $\mathbf{W}$ are two basic estimates for approximating other advanced estimates, i.e., unbiased variance $\hat{\sigma}_+^2 = \mathbf{W}(N-1)/N + \mathbf{B}/N$, pooled posterior variance estimate $\hat{\mathbf{V}} = \hat{\sigma}_+^2 + \mathbf{B}/(mN)$, the potential reduction scale factor $\hat{\mathbf{R}}$,

$$\frac{\mathbf{B}}{N} = \frac{1}{m-1} \sum_{j=1}^m (\bar{\boldsymbol{\theta}}_{j\cdot} - \bar{\boldsymbol{\theta}}_{\cdot\cdot})^2 \quad (1)$$

$$\mathbf{W} = \frac{1}{m(N-1)} \sum_{j=1}^m \sum_{t=1}^N (\boldsymbol{\theta}_{jt} - \bar{\boldsymbol{\theta}}_{j\cdot})^2 \quad (2)$$

and

$$\hat{\mathbf{R}} = \frac{\hat{\mathbf{V}}}{\mathbf{W}} \quad (3)$$

Generally, MCMC processes should proceed until $\hat{\mathbf{R}}$ approaches to 1, which means that the estimated variance has decrease sufficient enough and the simulated observations is close to the target distribution¹¹. Once the MCMC processes settles down, the posterior means are then estimated

$$\boldsymbol{\theta}_{\text{MAP}} = \frac{1}{N} \sum_i^N \hat{\boldsymbol{\theta}}_i \quad (4)$$

where $\hat{\boldsymbol{\theta}}_i$ is the estimation inferred from the i -th chain.

Modeling of interdiffusion coefficient: The interdiffusion coefficient matrices in Eq. (3) of the manuscript are in fact the thermodynamic and kinetic correlated terms¹⁻⁴,

$$\tilde{D}_{ij}^n = RT \left(M_i \phi_{ij}^n - x_i \sum_k M_k \phi_{kj}^n \right) + S \quad (5)$$

where R is the gas constant, T the absolute temperature. S denotes the contribution of

wind vacancy effect, for which different forms are available³⁻⁷. ϕ_{ij}^n is the thermodynamic factor given as

$$\phi_{ij}^n = \frac{x_k}{RT} \left(\frac{\partial \mu_k}{\partial x_j} - \frac{\partial \mu_k}{\partial x_n} \right) \quad (6)$$

For the atomic mobility M_k , the CALPHAD-type formalism proposed in Ref. ⁸ can be adopted,

$$M_k = \frac{1}{RT} \exp \left(\frac{\Phi_k}{RT} \right) {}^{\text{mg}}\Omega \quad (7)$$

where ${}^{\text{mg}}\Omega$ is a factor denoting the ferromagnetic contribution into the atomic mobility.

The mobility parameter Φ_k can be expanded with the Redlich-Kister polynomial

$$\begin{aligned} \Phi_k = & \sum_i x_i \Phi_k^i + \sum_i \sum_{j>i} x_i x_j \left[\sum_r^m {}^r\Phi_k^{i,j} (x_i - x_j)^r \right] + \\ & \sum_i \sum_{j>i} \sum_{k>j} x_i x_j x_k \left[\sum_r {}^r v_r^{ijk} \Phi_k^{i,j,k} \right] + \dots \end{aligned} \quad (8)$$

where Φ_k^i , ${}^r\Phi_k^{i,j}$ and ${}^r\Phi_k^{i,j,k}$ represent the contribution of unary, binary and ternary systems and v_r^{ijk} is represented as $x_r + (1 - x_i - x_j - x_k)/3$. In the present work, the interaction parameters, i.e., ${}^r\Phi_k^{i,j}$ and ${}^r\Phi_k^{i,j,k}$, are considered as the parameters of interest, i.e., θ , in Eqs. (2) and (3) of the manuscript. For detailed modeling of the inverse problem or the PDE-constrained optimization problem, one might refer to Refs. ^{9,10}.

Objective functions for variable-selection genetic algorithm: Regarding the relation between maximum value of the likelihood function and RSS value,

$$\ln(\hat{L}) = -\frac{N}{2} \ln \left(\frac{\text{RSS}}{N} \right) + C_1 \quad (9)$$

where N is the number of samples and C_1 is a constant, the objective function based on the AIC can be expressed as

$$\text{OBJ}_{\text{AIC}} = 2K + N \ln \left(\frac{\text{RSS}}{N} \right) \quad (10)$$

or Bayesian information criterion,

$$\text{OBJ}_{\text{BIC}} = K \ln(N) + N \ln \left(\frac{\text{RSS}}{N} \right) \quad (11)$$

where N is the number of samples, K is the number of the effective parameters, and $\hat{L}$ is maximum value of the likelihood function. The corrected form of AIC, i.e., AICc, for dataset with small sample size can be expressed as

$$\text{AICc} = \text{AIC} + \frac{2K(K+1)}{N-K-1} \quad (12)$$

where N is the number of observations. Generally, the AIC tends to overparameterize as the pretty low penalty on the sample sizes is imposed, and AICc is often adopted as

a better alternative.

$$\text{OBJ}_{\text{AICc}} = 2K + N \ln \left(\frac{\text{RSS}}{N} \right) + \frac{2K(K+1)}{N-K-1} \quad (13)$$

Benchmark over fully implicit finite difference method: For a system with M components, the related diffusion equation of the p -th component at the i -th grid can be discretized as

$$\frac{c_{p,i}^{t+1} - c_{p,i}^t}{\Delta t} = \sum_{q=1}^{M-1} \left[D_{pq,i+1/2}^{t+1} \frac{c_{q,i+1}^{t+1} - c_{q,i}^{t+1}}{h_i^+} - D_{pq,i-1/2}^{t+1} \frac{c_{q,i}^{t+1} - c_{q,i-1}^{t+1}}{h_i^-} \right] / \left[\frac{1}{2} (h_i^- + h_i^+) \right] \quad (14)$$

$$\frac{1}{\Delta t} c_{p,i}^{t+1} - \frac{1}{\Delta t} c_{p,i}^t = \sum_{q=1}^{M-1} \left[D_{pq,i+1/2}^{t+1} \frac{c_{q,i+1}^{t+1} - c_{q,i}^{t+1}}{h_i^+} - D_{pq,i-1/2}^{t+1} \frac{c_{q,i}^{t+1} - c_{q,i-1}^{t+1}}{h_i^-} \right] / \left[\frac{1}{2} (h_i^- + h_i^+) \right] \quad (15)$$

$$\begin{aligned} \frac{1}{\Delta t} c_{p,i}^{t+1} - \frac{1}{\Delta t} c_{p,i}^t &= \left[D_{pp,i+1/2}^{t+1} \frac{c_{p,i+1}^{t+1} - c_{p,i}^{t+1}}{h_i^+} - D_{pp,i-1/2}^{t+1} \frac{c_{p,i}^{t+1} - c_{p,i-1}^{t+1}}{h_i^-} \right] / \left[\frac{1}{2} (h_i^- + h_i^+) \right] \\ &= \sum_{q \neq p}^{M-1} \left[D_{pq,i+1/2}^{t+1} \frac{c_{q,i+1}^{t+1} - c_{q,i}^{t+1}}{h_i^+} - D_{pq,i-1/2}^{t+1} \frac{c_{q,i}^{t+1} - c_{q,i-1}^{t+1}}{h_i^-} \right] / \left[\frac{1}{2} (h_i^- + h_i^+) \right] \end{aligned} \quad (16)$$

$$\begin{aligned} &-c_{p,i-1}^{t+1} \left[\frac{2D_{pp,i-1/2}^{t+1}}{h_i^- (h_i^- + h_i^+)} \right] + c_{p,i}^{t+1} \left[\frac{1}{\Delta t} + \frac{2D_{pp,i+1/2}^{t+1}}{h_i^+ (h_i^- + h_i^+)} + \frac{2D_{pp,i-1/2}^{t+1}}{h_i^- (h_i^- + h_i^+)} \right] - c_{p,i+1}^{t+1} \left[\frac{2D_{pp,i+1/2}^{t+1}}{h_i^+ (h_i^- + h_i^+)} \right] \\ &= \frac{1}{\Delta t} c_{p,i}^t + \sum_{q \neq p}^{M-1} \left[\frac{2D_{pq,i-1/2}^{t+1}}{h_i^- (h_i^- + h_i^+)} c_{q,i-1}^{t+1} - \left(\frac{2D_{pq,i+1/2}^{t+1}}{h_i^+ (h_i^- + h_i^+)} - \frac{2D_{pq,i-1/2}^{t+1}}{h_i^- (h_i^- + h_i^+)} \right) c_{q,i}^{t+1} \right. \\ &\quad \left. + \frac{2D_{pq,i+1/2}^{t+1}}{h_i^+ (h_i^- + h_i^+)} c_{q,i+1}^{t+1} \right] \end{aligned} \quad (17)$$

$$A_{pq,i,i}^{t+1} = \frac{2D_{pp,i+1/2}^{t+1}}{h_i^+ (h_i^- + h_i^+)} + \frac{2D_{pp,i-1/2}^{t+1}}{h_i^- (h_i^- + h_i^+)} \quad (18)$$

$$A_{pq,i,i-1}^{t+1} = \frac{2D_{pp,i-1/2}^{t+1}}{h_i^- (h_i^- + h_i^+)} \quad (19)$$

$$A_{pq,i,i+1}^{t+1} = \frac{2D_{pp,i+1/2}^{t+1}}{h_i^+ (h_i^- + h_i^+)} \quad (20)$$

$$b_{p,i} = \frac{1}{\Delta t} c_{p,i}^t + \sum_{q \neq p}^{M-1} \left[\frac{2D_{pq,i-1/2}^{t+1}}{h_i^- (h_i^- + h_i^+)} c_{q,i-1}^{t+1} - \left(\frac{2D_{pq,i+1/2}^{t+1}}{h_i^+ (h_i^- + h_i^+)} - \frac{2D_{pq,i-1/2}^{t+1}}{h_i^- (h_i^- + h_i^+)} \right) c_{q,i}^{t+1} + \frac{2D_{pq,i+1/2}^{t+1}}{h_i^+ (h_i^- + h_i^+)} c_{q,i+1}^{t+1} \right] \quad (21)$$

For zero-flux boundary condition,

$$A_{pq,0,0}^{t+1} = 1, A_{ij,0,1}^{t+1} = -1, b_{p,0}^t = 0 \quad (22)$$

and

$$A_{pq,N-1,N-1}^{t+1} = 1, A_{pq,N-1,N-2}^{t+1} = -1, b_{p,N-1}^t = 0. \quad (23)$$

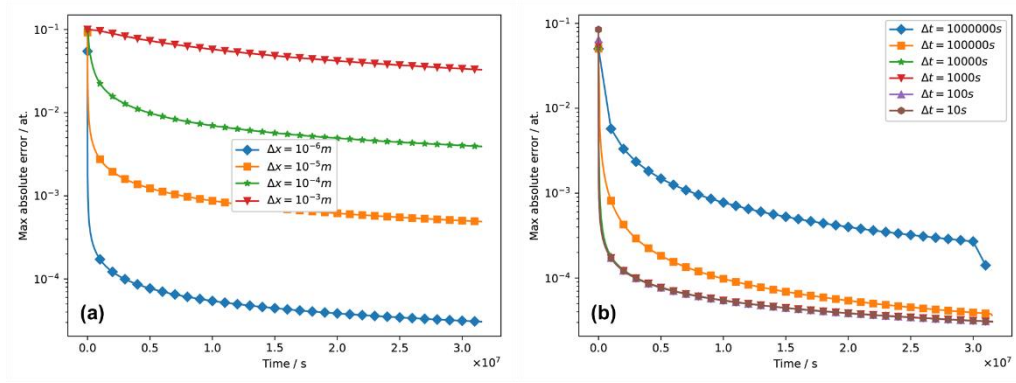
A benchmark for the implicit finite difference scheme is illustrated in Supplementary Figure 1, where a hypothetical binary diffusion couple with composition-dependent interdiffusion coefficient is considered. The overall annealing time for the diffusion couple is set to be 1 year. A solution of high resolution is firstly obtained by means of explicit finite difference method with $\Delta x = 10^{-6}$ m and $\Delta t = 1$ s. Tests are conducted from two aspects, i.e., with different step sizes of space or time. In the first case, the step size of time for the implicit finite difference scheme is fixed at $\Delta t = 1000$ s, while Δx varies from 10^{-6} m to 10^{-3} m. The deviation between the results using different step sizes of space is then compared with the solution of fine resolution, as shown in Supplementary Figure 1a. In the second case, the step size of space is fixed at $\Delta x = 10^{-6}$ m, while the Δt varies from 10 s to 10^6 s. Deviation against the solution of high resolution is presented in Supplementary Figure 1b. As the time evolves, the deviation shrinks for each sequence in Supplementary Figure 1a. Similar trending is observed in Supplementary Figure 1b, where the fixed step size of space is adopted while the step size of time varies. In case that Δt is fixed, the simulation result using step size of space, i.e., $\Delta x = 10^{-6}$ m, achieve the least deviation to the solution of high resolution. As the step size of space is fixed, $\Delta t = 1000$ s and $\Delta t = 10000$ s are able to achieve result of reasonable accuracy. To sum up, the implicit scheme is robust with respect to a wide range of step sizes of time and space, while $\Delta x = 10^{-6}$ m and $\Delta t = 1000$ s are adopted as the default setting for the solver to the diffusion equations.

Algorithm 1. Solve Eqs. (17)-(23)

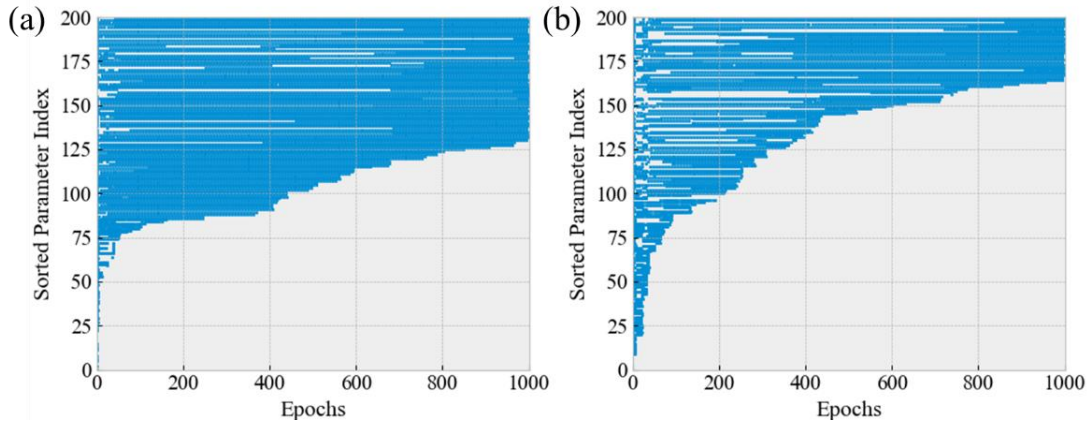
1. $\mathbf{c}_1^{t+1,0}, \dots, \mathbf{c}_{M-1}^{t+1,0} \Leftarrow \mathbf{c}_1^t, \dots, \mathbf{c}_{M-1}^t$
 2. for $p=1$ to $M-1$ do
 3. $\mathbf{D}_{pq}^{t+1} \Leftarrow f(\mathbf{c}_1^{t+1,m-1}, \dots, \mathbf{c}_{M-1}^{t+1,m-1})$ for all grid node
 4. for $q=1$ to $M-1$ do
 5. $\mathbf{c}_p^{t+1,m} \Leftarrow \text{TDMA}(\mathbf{A}_{pq}, \mathbf{b}_p)$
 6. end for
 7. if $\max(|\mathbf{c}_p^{t+1,m} - \mathbf{c}_p^{t+1,m-1}|) \leq \epsilon$ for $p=1$ to $M-1$ then
 8. break
 9. end if
 10. end for
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Note: f refers to the interdiffusion coefficient functions; ϵ is the pre-defined tolerance

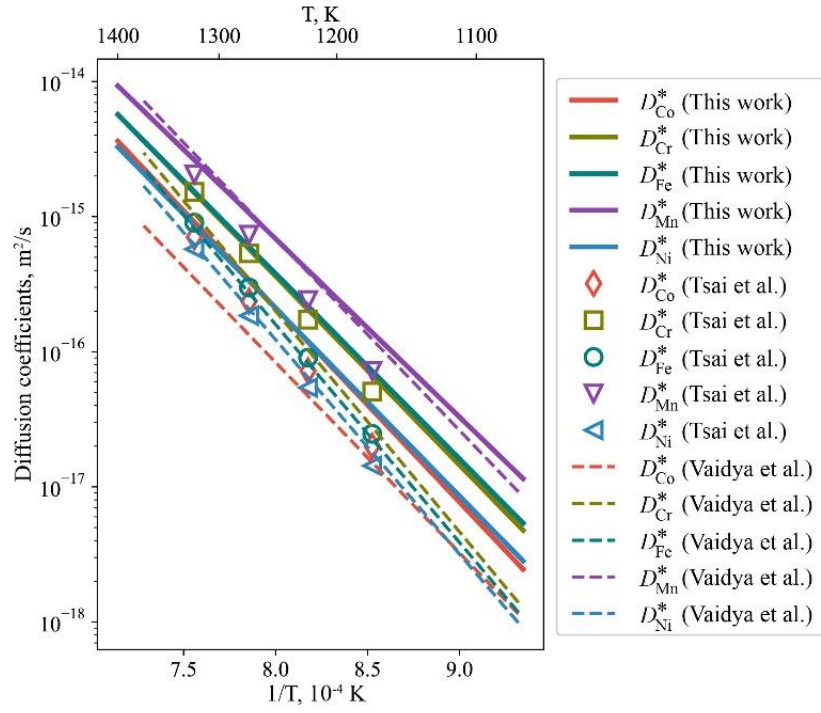
Supplementary Figures



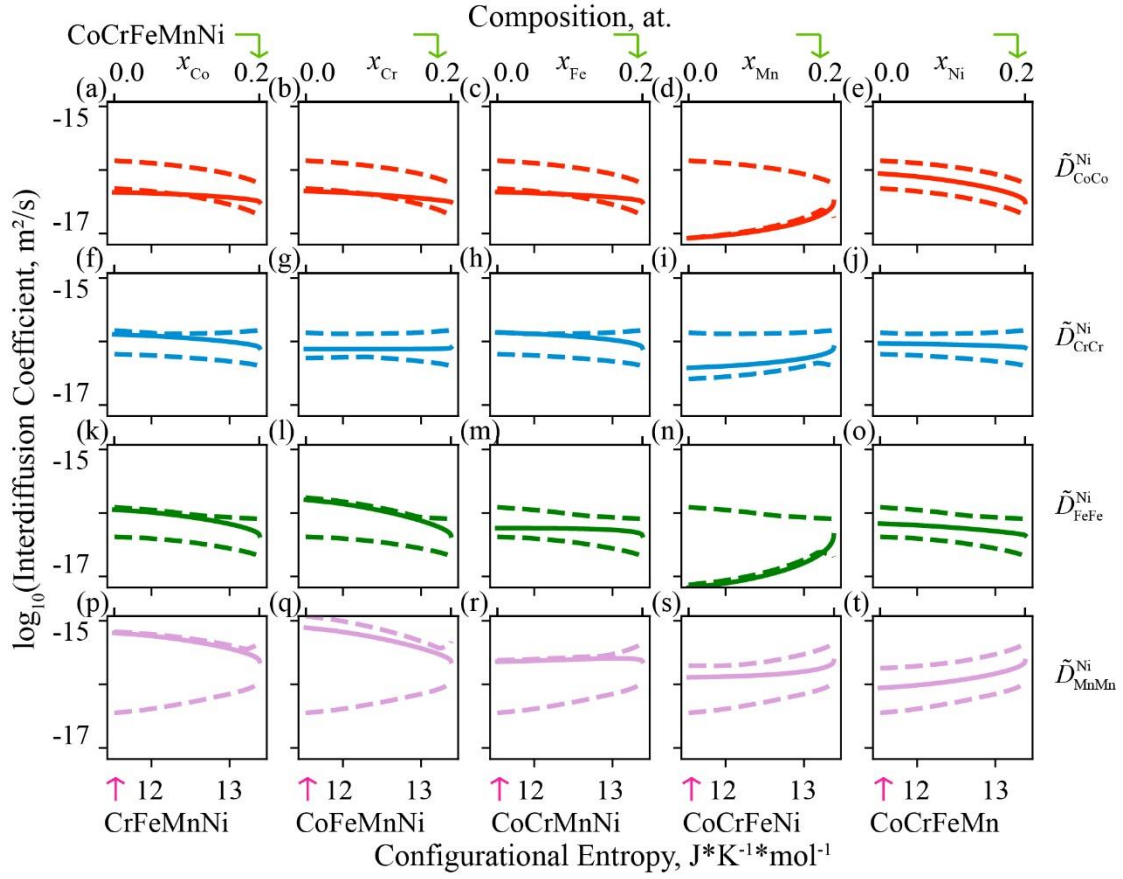
Supplementary Figure 1: Benchmarks on the implicit finite difference methods. Convergence sequence of the implicit finite difference scheme on simulating a hypothetical binary system ($D = 10^{-14} + 10^{-15}c, \text{m}^2/\text{s}$, annealed for one year) using different time and space step sizes (a) fixed $\Delta t = 1000$ s; (b) fixed $\Delta x = 10^{-6}$ m.



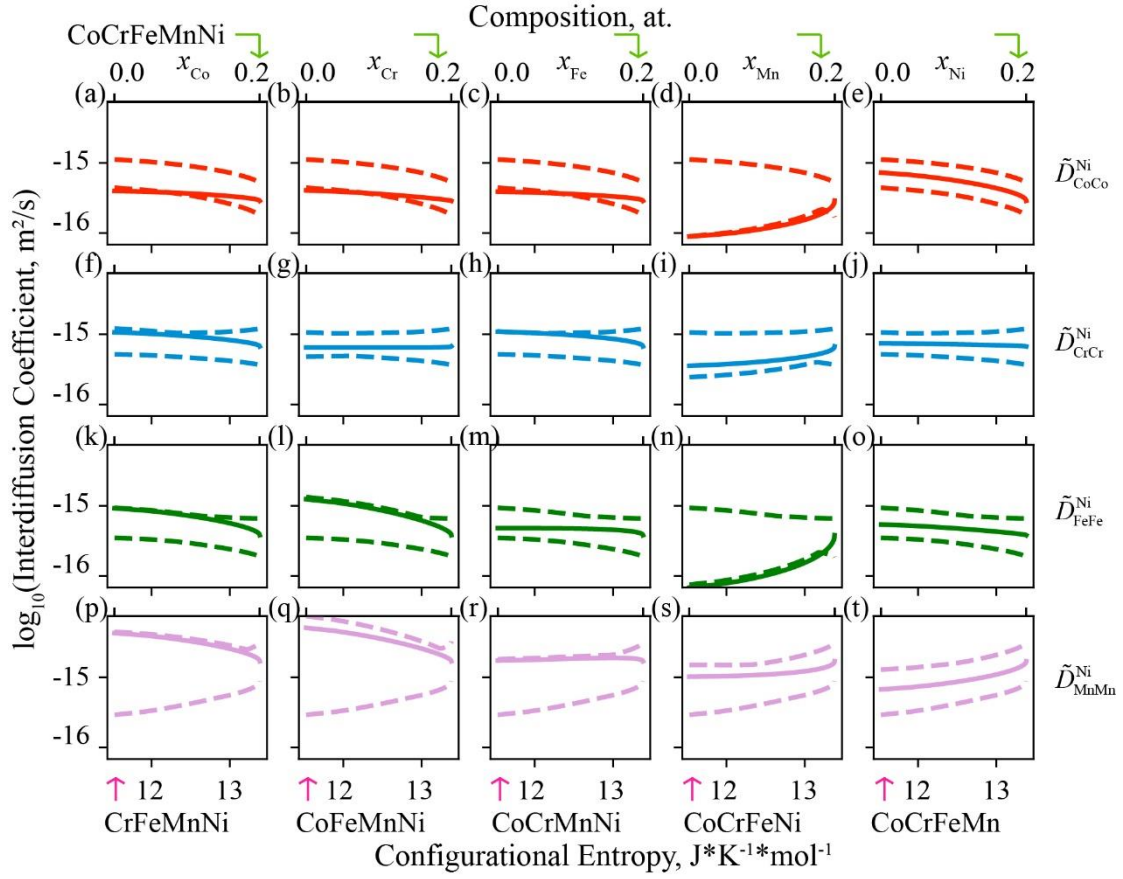
Supplementary Figure 2: Selection roadmap of variable-selection genetic algorithm. The effective parameters of interest are selected based on (a) AIC and (b) BIC.



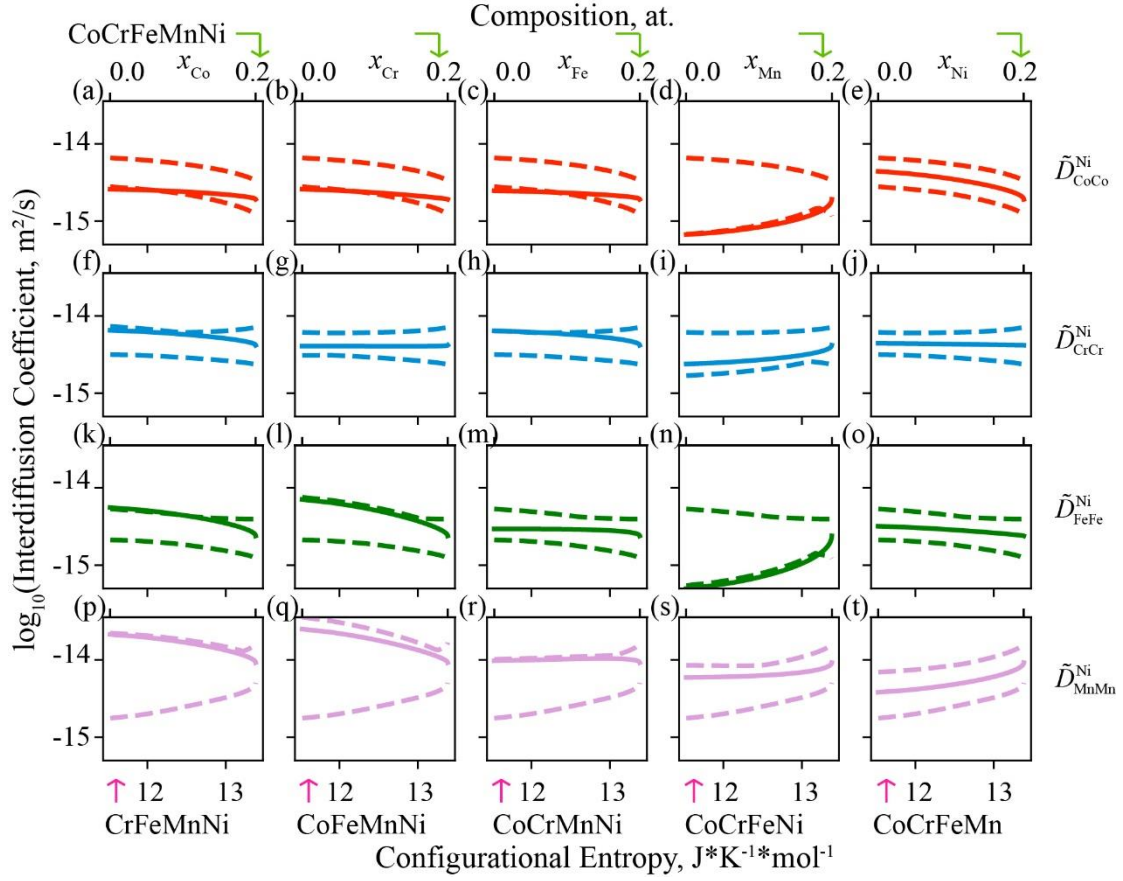
Supplementary Figure 3: Comparison of the tracer diffusion coefficients in fcc CoCrFeMnNi HEAs. The tracer diffusion coefficients are ported from the present work, Tsai et al.¹² and Vaidya et al.^{13,14}



Supplementary Figure 4: Projections of interdiffusion coefficients at along different composition coordinates. The dash lines refer to the bounds of the related interdiffusion coefficients ($\tilde{D}_{\text{CoCo}}^{\text{Ni}}$, $\tilde{D}_{\text{CrCr}}^{\text{Ni}}$, $\tilde{D}_{\text{FeFe}}^{\text{Ni}}$, $\tilde{D}_{\text{MnMn}}^{\text{Ni}}$) at 1173 K, while the solid line is related to interdiffusion coefficients due to the maximum a-posterior.



Supplementary Figure 5: Projections of interdiffusion coefficients at along different composition coordinates. The dash lines refer to the bounds of the related interdiffusion coefficients ($\tilde{D}_{\text{CoCo}}^{\text{Ni}}$, $\tilde{D}_{\text{CrCr}}^{\text{Ni}}$, $\tilde{D}_{\text{FeFe}}^{\text{Ni}}$, $\tilde{D}_{\text{MnMn}}^{\text{Ni}}$) at 1273 K, while the solid line is related to interdiffusion coefficients due to the maximum a-posterior.



Supplementary Figure 6: Projections of interdiffusion coefficients at along different composition coordinates. The dash lines refer to the bounds of the related interdiffusion coefficients ($\tilde{D}_{\text{CoCo}}^{\text{Ni}}, \tilde{D}_{\text{CrCr}}^{\text{Ni}}, \tilde{D}_{\text{FeFe}}^{\text{Ni}}, \tilde{D}_{\text{MnMn}}^{\text{Ni}}$) at 1373 K, while the solid line is related to interdiffusion coefficients due to the maximum a-posterior.

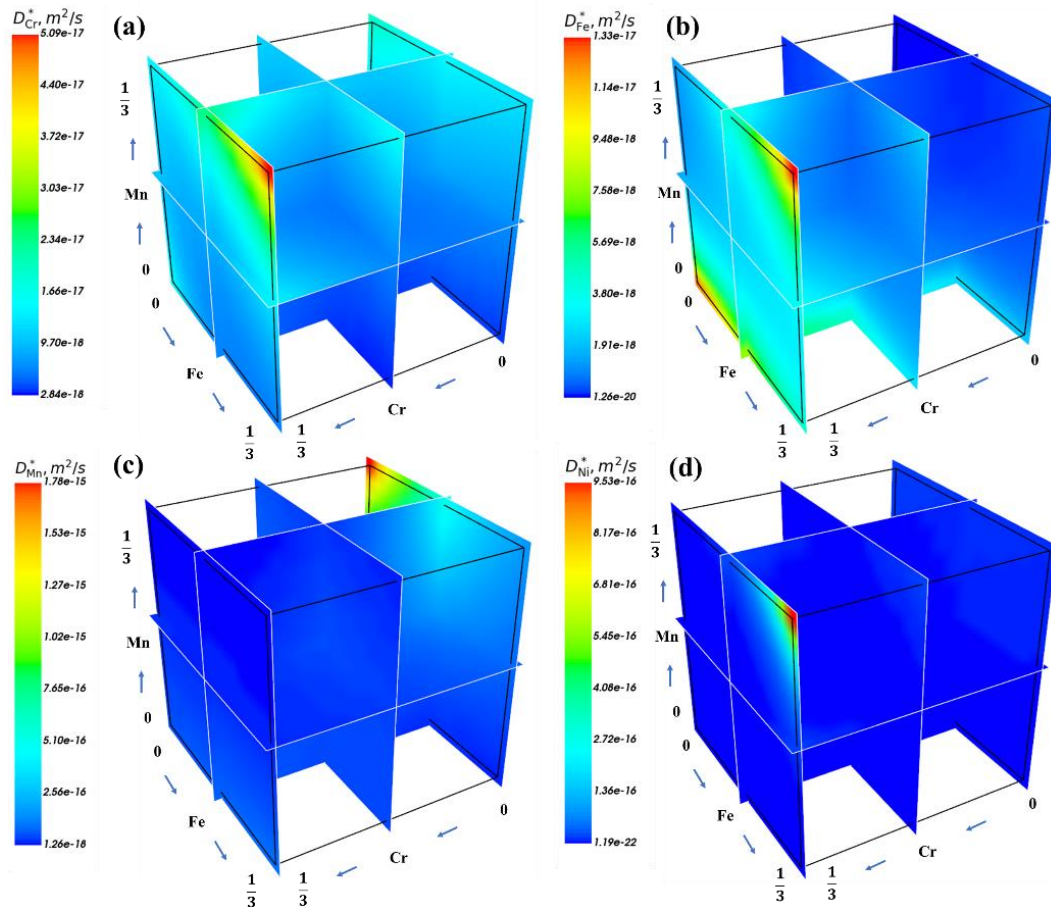
Supplementary Tables

Supplementary Table 1: Activation energies and frequency factors of the tracer diffusion coefficients. Quantities related to tracer diffusion coefficients of the CoCrFeMnNi system and its corresponding quaternary systems measured in the present work, where D_0 stands for $\times 10^{-4}\text{m}^2/\text{s}$ and Q stands for kJ/mol.

System	D_{Co}^*		D_{Cr}^*		D_{Fe}^*		D_{Mn}^*		D_{Ni}^*	
	D_0	Q	D_0	Q	D_0	Q	D_0	Q	D_0	Q
CoCrFeMnNi	0.68	275.4	0.55	267.6	0.36	262.9	0.25	252.7	0.28	266.4
CoCrFeMn	0.47	267.3	0.33	252.2	0.21	237.1	0.16	265.1	-	-
CoCrFeNi	1.19	292.9	0.91	282.3	0.54	278.4	-	-	0.40	289.1
CoCrMnNi	0.62	273.4	0.41	257.4	-	-	0.41	258.0	0.28	265.9
CoFeMnNi	0.73	268.5	-	-	0.33	259.2	0.21	232.6	0.24	256.1
CrFeMnNi	-	-	0.74	264.2	0.54	278.0	0.21	250.5	0.29	266.7

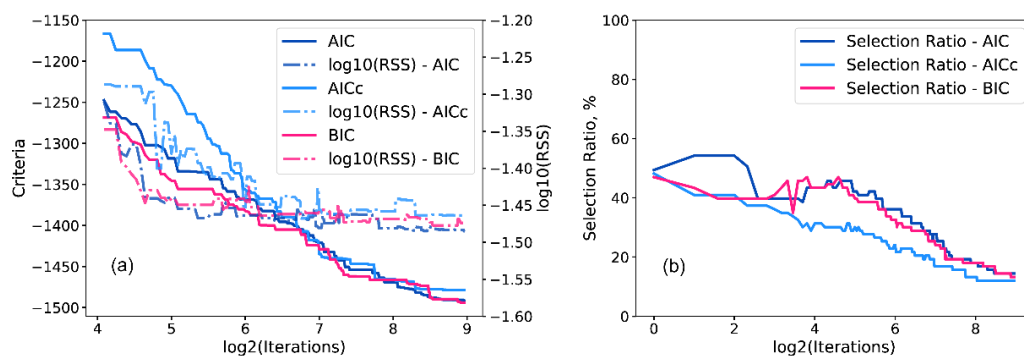
Supplementary Discussion

Diffusion descriptions of CoCrFeMnNi system and its subsystems: Among the fcc CoCrFeMnNi system and its sub-systems, fcc CrFeMnNi alloy is considered as one of the alternatives with promising radiation resistance¹⁵. However, measurement of the related systems is missing currently. With the established diffusion database, the diffusion description of the fcc CrFeMnNi alloy is thus predicted, as illustrated in Supplementary Figure 7, where the effective tracer diffusion coefficients are presented. For the components, i.e., Co, Fe, Ni, the effective tracer diffusion coefficients achieve larger value around the center of composition space. The effective tracer diffusion coefficients of Mn decrease significantly with the addition of Fe and Cr. Around the equal atomic constituents for the fcc CrFeMnNi alloy, the scale of effective tracer diffusion coefficient ranks as $D_{\text{Ni}}^* > D_{\text{Cr}}^* > D_{\text{Fe}}^* > D_{\text{Mn}}^*$.

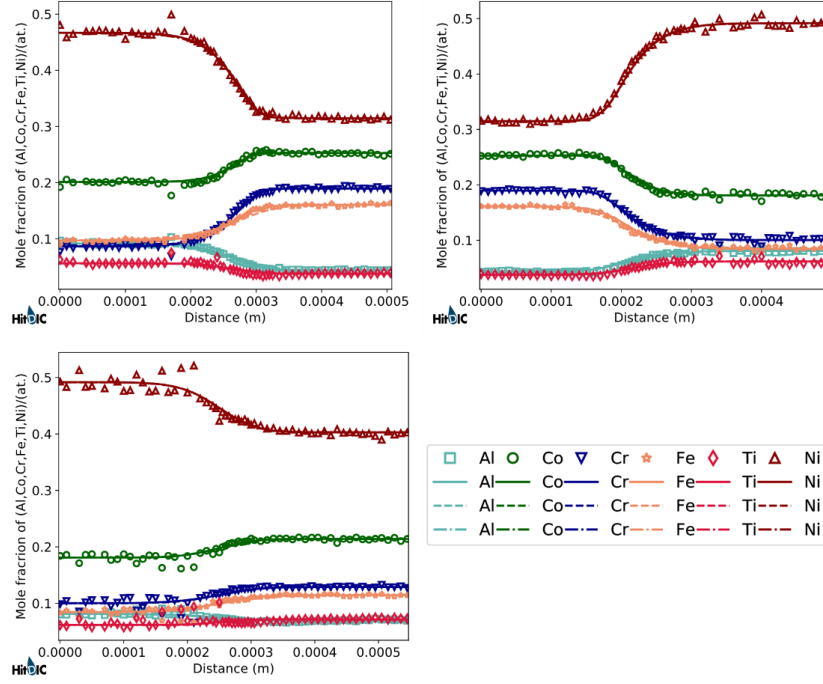


Supplementary Figure 7: Illustration of the effective tracer diffusion coefficients of fcc CrFeMnNi HEAs at 1073 K. (a) Tracer diffusivity of Cr; (b) Tracer diffusivity of Fe; (c) Tracer diffusivity of Mn; (d) Tracer diffusivity of Ni.

Benchmark over the variable-selection genetic algorithm: A benchmark test on the efficiency of different criteria is demonstrated with the fcc Al-Co-Cr-Fe-Ni-Ti high-entropy superalloys, where 3 diffusion couples¹⁶ and 83 parameters of interest are concerned. Good agreement between the predictions and the observations indicates that the proposed optimization algorithm is capable of recovering the satisfactory estimation of the concerned parameters, as is illustrated in the supplementary. Convergence behavior of the algorithm adopting different criteria is presented in Supplementary Figure 8, where the scores of different information criteria, residual summation of square and the selection ratios are superimposed. The scores of AIC and BIC behave similarly, while the AICc tends to converge slower at the early stage. Similar convergence trend is observed among the sequence of RSS, where AIC or BIC leads to faster convergence rates. The selection efficiencies at the final stages are similar, which are close to 14%. However, the convergence sequence of the selection ratio using AICc evolve rather smoothly, as is shown in Supplementary Figure 8b. That is, AIC or BIC tends to induce the optimizer to explore the parameter space with better fitting goodness at the early stage, while they turn to explore the parameter space of high selection efficiency during the successive stage. Overall, the difference of fitting goodness among model-predicted composition profiles due to different selection criteria are trivial, implying the validity of the proposed algorithm and selection criteria, as indicated in Supplementary Figure 9. However, the AICc tends to penal fairly on the number of effective parameters and fitting goodness, as the trending of RSS and selection ratio evolve quite smoothly.



Supplementary Figure 8: Convergence sequences of the variable-selection genetic algorithm. Sequences of selection criteria, RSS and selection ratios for a dataset with 3 diffusion couples of a senary high entropy superalloy (Al-Co-Cr-Fe-Ni-Ti) and 83 parameters of interest.



Supplementary Figure 9: Comparison of model-predicted and experimental composition profiles. Experimental data refers to fcc AlCoCrFeNiTi high entropy superalloys, while the predictions are based on the optimization results using different types of criteria.

Supplementary References

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Supplementary Table 2: Lists of the parameters and their estimations

Parameter	Notion	AIC	BIC	ReL1	ReL2	MCMC
$0\Phi_{\text{Co,Cr}}$	A0	-160772.7	0.0	-	-	-
$0\Phi_{\text{Co,Fe}}$	A1	166461.2	0.0	-	-	-
$0\Phi_{\text{Co,Mn}}$	A2	0.0	30572.5	26611.3	46618.7	-5065.4
$0\Phi_{\text{Co,Ni}}$	A3	0.0	0.0	-	-	-
$0\Phi_{\text{Cr,Fe}}$	A4	0.0	0.0	-	-	-
$0\Phi_{\text{Cr,Mn}}$	A5	0.0	0.0	-	-	-
$0\Phi_{\text{Cr,Ni}}$	A6	0.0	-195349.1	-221801.8	-249664.3	-224317.8
$0\Phi_{\text{Fe,Mn}}$	A7	155181.9	0.0	-	-	-
$0\Phi_{\text{Fe,Ni}}$	A8	-138214.1	0.0	-	-	-
$0\Phi_{\text{Mn,Ni}}$	A9	0.0	0.0	-	-	-
$0\Phi_{\text{Co,Cr}}$	A10	-12463.4	0.0	-	-	-
$0\Phi_{\text{Co,Fe}}$	A11	0.0	-175408.9	-127136.2	-132104.5	-119607.6
$0\Phi_{\text{Co,Mn}}$	A12	0.0	0.0	-	-	-
$0\Phi_{\text{Cr,Ni}}$	A13	0.0	0.0	-	-	-
$0\Phi_{\text{Cr,Fe}}$	A14	0.0	0.0	-	-	-
$0\Phi_{\text{Cr,Mn}}$	A15	0.0	0.0	-	-	-
$0\Phi_{\text{Cr,Ni}}$	A16	0.0	-33612.1	-112164.3	-90008.5	-74623.3
$0\Phi_{\text{Fe,Mn}}$	A17	0.0	0.0	-	-	-
$0\Phi_{\text{Fe,Ni}}$	A18	0.0	0.0	-	-	-
$0\Phi_{\text{Mn,Ni}}$	A19	0.0	0.0	-	-	-
$0\Phi_{\text{Co,Cr}}$	A20	0.0	0.0	-	-	-
$0\Phi_{\text{Co,Fe}}$	A21	111877.4	0.0	-	-	-
$0\Phi_{\text{Co,Mn}}$	A22	0.0	0.0	-	-	-
$0\Phi_{\text{Co,Ni}}$	A23	151757.8	0.0	-	-	-
$0\Phi_{\text{Cr,Fe}}$	A24	-408313.0	-163256.8	-176617.4	-220861.8	-159661.5
$0\Phi_{\text{Cr,Mn}}$	A25	0.0	0.0	-	-	-
$0\Phi_{\text{Cr,Ni}}$	A26	0.0	0.0	-	-	-
$0\Phi_{\text{Fe,Mn}}$	A27	0.0	0.0	-	-	-
$0\Phi_{\text{Fe,Ni}}$	A28	0.0	0.0	-	-	-
$0\Phi_{\text{Mn,Ni}}$	A29	-265039.1	130877.7	105566.4	95294.2	67438.2
$0\Phi_{\text{Co,Cr}}$	A30	0.0	0.0	-	-	-
$0\Phi_{\text{Co,Fe}}$	A31	0.0	0.0	-	-	-
$0\Phi_{\text{Co,Mn}}$	A32	120941.2	293756.1	231384.3	256964.1	-5099.0
$0\Phi_{\text{Co,Ni}}$	A33	0.0	-254162.6	-252551.3	-250537.1	70728.3
$0\Phi_{\text{Cr,Fe}}$	A34	0.0	0.0	-	-	-
$0\Phi_{\text{Cr,Mn}}$	A35	-93499.8	0.0	-	-	-

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Supplementary Table 2 – Lists of the parameters and their estimations (Continued)

Parameter	Notion	AIC	BIC	ReL1	ReL2	MCMC
$0\Phi_{\text{Mn}}^{\text{Cr,Ni}}$	A36	0.0	0.0	-	-	-
$0\Phi_{\text{Mn}}^{\text{Fe,Mn}}$	A37	93682.9	0.0	-	-	-
$0\Phi_{\text{Mn}}^{\text{Fe,Ni}}$	A38	0.0	0.0	-	-	-
$0\Phi_{\text{Mn}}^{\text{Mn,Ni}}$	A39	-44689.9	0.0	-	-	-
$0\Phi_{\text{Ni}}^{\text{Co,Cr}}$	A40	0.0	0.0	-	-	-
$0\Phi_{\text{Ni}}^{\text{Co,Fe}}$	A41	0.0	0.0	-	-	-
$0\Phi_{\text{Ni}}^{\text{Co,Mn}}$	A42	0.0	0.0	-	-	-
$0\Phi_{\text{Ni}}^{\text{Co,Ni}}$	A43	21441.7	0.0	-	-	-
$0\Phi_{\text{Ni}}^{\text{Cr,Fe}}$	A44	-354064.9	0.0	-	-	-
$0\Phi_{\text{Ni}}^{\text{Cr,Mn}}$	A45	-528491.2	-668475.3	-425500.5	-274304.2	-200146.1
$0\Phi_{\text{Ni}}^{\text{Cr,Ni}}$	A46	0.0	0.0	-	-	-
$0\Phi_{\text{Ni}}^{\text{Fe,Mn}}$	A47	-224017.3	0.0	-	-	-
$0\Phi_{\text{Ni}}^{\text{Fe,Ni}}$	A48	0.0	-197631.8	-177893.1	-160907.0	-93045.4
$0\Phi_{\text{Ni}}^{\text{Mn,Ni}}$	A49	247766.1	261395.3	238098.1	122552.5	131669.3
$0\Phi_{\text{Co}}^{\text{Co,Cr,Fe}}$	A50	0.0	0.0	-	-	-
$1\Phi_{\text{Co}}^{\text{Co,Cr,Fe}}$	A51	0.0	0.0	-	-	-
$2\Phi_{\text{Co}}^{\text{Co,Cr,Fe}}$	A52	-187493.9	0.0	-	-	-
$0\Phi_{\text{Co}}^{\text{Co,Cr,Mn}}$	A53	0.0	0.0	-	-	-
$1\Phi_{\text{Co}}^{\text{Co,Cr,Mn}}$	A54	-499554.4	0.0	-	-	-
$2\Phi_{\text{Co}}^{\text{Co,Cr,Mn}}$	A55	0.0	0.0	-	-	-
$0\Phi_{\text{Co}}^{\text{Co,Cr,Ni}}$	A56	98785.4	0.0	-	-	-
$1\Phi_{\text{Co}}^{\text{Co,Cr,Ni}}$	A57	0.0	-129016.1	-379510.5	-4473.9	-415332.6
$2\Phi_{\text{Co}}^{\text{Co,Cr,Ni}}$	A58	0.0	0.0	-	-	-
$0\Phi_{\text{Co}}^{\text{Co,Fe,Mn}}$	A59	-246643.1	0.0	-	-	-
$1\Phi_{\text{Co}}^{\text{Co,Fe,Mn}}$	A60	0.0	0.0	-	-	-
$2\Phi_{\text{Co}}^{\text{Co,Fe,Mn}}$	A61	0.0	0.0	-	-	-
$0\Phi_{\text{Co}}^{\text{Co,Fe,Ni}}$	A62	0.0	0.0	-	-	-
$1\Phi_{\text{Co}}^{\text{Co,Fe,Ni}}$	A63	0.0	0.0	-	-	-
$2\Phi_{\text{Co}}^{\text{Co,Fe,Ni}}$	A64	0.0	0.0	-	-	-
$0\Phi_{\text{Co}}^{\text{Co,Mn,Ni}}$	A65	-271618.7	0.0	-	-	-
$1\Phi_{\text{Co}}^{\text{Co,Mn,Ni}}$	A66	0.0	-242547.6	-99676.5	118255.6	-480462.9
$2\Phi_{\text{Co}}^{\text{Co,Mn,Ni}}$	A67	-582269.3	0.0	-	-	-
$0\Phi_{\text{Co}}^{\text{Cr,Fe,Mn}}$	A68	0.0	0.0	-	-	-
$1\Phi_{\text{Co}}^{\text{Cr,Fe,Mn}}$	A69	0.0	-308544.9	31579.6	-29382.3	72237.9
$2\Phi_{\text{Co}}^{\text{Cr,Fe,Mn}}$	A70	-266247.6	0.0	-	-	-
$0\Phi_{\text{Co}}^{\text{Cr,Fe,Ni}}$	A71	-711108.4	0.0	-	-	-
$1\Phi_{\text{Co}}^{\text{Cr,Fe,Ni}}$	A72	0.0	0.0	-	-	-

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Supplementary Table 2 – Lists of the parameters and their estimations (Continued)

Parameter	Notion	AIC	BIC	ReL1	ReL2	MCMC
$2\Phi_{\text{Co,Fe,Ni}}$	A73	0.0	0.0	-	-	-
$0\Phi_{\text{Cr,Mn,Ni}}$	A74	0.0	0.0	-	-	-
$1\Phi_{\text{Co,Cr,Mn,Ni}}$	A75	0.0	0.0	-	-	-
$2\Phi_{\text{Co,Cr,Mn,Ni}}$	A76	0.0	0.0	-	-	-
$0\Phi_{\text{Fe,Mn,Ni}}$	A77	0.0	0.0	-	-	-
$1\Phi_{\text{Fe,Mn,Ni}}$	A78	0.0	0.0	-	-	-
$2\Phi_{\text{Fe,Mn,Ni}}$	A79	-281085.2	0.0	-	-	-
$0\Phi_{\text{Co,Co,Cr,Fe}}$	A80	-620336.9	0.0	-	-	-
$1\Phi_{\text{Co,Co,Cr,Fe}}$	A81	0.0	0.0	-	-	-
$2\Phi_{\text{Co,Co,Cr,Fe}}$	A82	0.0	0.0	-	-	-
$0\Phi_{\text{Co,Co,Cr,Mn}}$	A83	0.0	0.0	-	-	-
$1\Phi_{\text{Co,Co,Cr,Mn}}$	A84	0.0	0.0	-	-	-
$2\Phi_{\text{Co,Co,Cr,Mn}}$	A85	-622149.7	0.0	-	-	-
$0\Phi_{\text{Co,Co,Cr,Ni}}$	A86	-306127.9	0.0	-	-	-
$1\Phi_{\text{Co,Co,Cr,Ni}}$	A87	-371118.2	-155938.7	217083.7	-263763.4	-320802.8
$2\Phi_{\text{Co,Co,Cr,Ni}}$	A88	0.0	0.0	-	-	-
$0\Phi_{\text{Co,Co,Fe,Mn}}$	A89	0.0	0.0	-	-	-
$1\Phi_{\text{Co,Co,Fe,Mn}}$	A90	0.0	0.0	-	-	-
$2\Phi_{\text{Co,Co,Fe,Mn}}$	A91	6335.4	-344262.7	-55566.4	39971.9	-533787.0
$0\Phi_{\text{Co,Co,Fe,Ni}}$	A92	0.0	109594.7	112078.9	164178.5	243389.4
$1\Phi_{\text{Co,Co,Fe,Ni}}$	A93	-718493.7	0.0	-	-	-
$2\Phi_{\text{Co,Co,Fe,Ni}}$	A94	0.0	0.0	-	-	-
$0\Phi_{\text{Co,Co,Mn,Ni}}$	A95	0.0	0.0	-	-	-
$1\Phi_{\text{Co,Co,Mn,Ni}}$	A96	0.0	0.0	-	-	-
$2\Phi_{\text{Co,Co,Mn,Ni}}$	A97	0.0	0.0	-	-	-
$0\Phi_{\text{Co,Co,Fe,Mn}}$	A98	184924.3	0.0	-	-	-
$1\Phi_{\text{Co,Co,Fe,Mn}}$	A99	0.0	0.0	-	-	-
$2\Phi_{\text{Co,Co,Fe,Mn}}$	A100	0.0	0.0	-	-	-
$0\Phi_{\text{Co,Co,Fe,Ni}}$	A101	-352386.5	0.0	-	-	-
$1\Phi_{\text{Co,Co,Fe,Ni}}$	A102	0.0	0.0	-	-	-
$2\Phi_{\text{Co,Co,Fe,Ni}}$	A103	0.0	0.0	-	-	-
$0\Phi_{\text{Co,Co,Mn,Ni}}$	A104	0.0	0.0	-	-	-
$1\Phi_{\text{Co,Co,Mn,Ni}}$	A105	0.0	-638330.1	32049.6	81127.9	-554963.1
$2\Phi_{\text{Co,Co,Mn,Ni}}$	A106	0.0	0.0	-	-	-
$0\Phi_{\text{Fe,Mn,Ni}}$	A107	0.0	0.0	-	-	-
$1\Phi_{\text{Fe,Mn,Ni}}$	A108	-37036.1	0.0	-	-	-
$2\Phi_{\text{Fe,Mn,Ni}}$	A109	0.0	0.0	-	-	-

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Supplementary Table 2 – Lists of the parameters and their estimations (Continued)

Parameter	Notion	AIC	BIC	ReL1	ReL2	MCMC
$0\Phi_{\text{Co,Cr,Fe}}$	A110	-25152.6	0.0	-	-	-
$1\Phi_{\text{Co,Cr,Fe}}$	A111	0.0	0.0	-	-	-
$2\Phi_{\text{Co,Cr,Fe}}$	A112	0.0	0.0	-	-	-
$0\Phi_{\text{Co,Cr,Mn}}$	A113	-169299.3	0.0	-	-	-
$1\Phi_{\text{Co,Cr,Mn}}$	A114	0.0	0.0	-	-	-
$2\Phi_{\text{Co,Cr,Mn}}$	A115	0.0	-766430.7	-354400.6	48431.4	-308992.2
$0\Phi_{\text{Co,Cr,Ni}}$	A116	-244226.1	-611340.3	-189373.8	-41467.3	-1162293.4
$1\Phi_{\text{Co,Cr,Ni}}$	A117	0.0	0.0	-	-	-
$2\Phi_{\text{Co,Cr,Ni}}$	A118	0.0	0.0	-	-	-
$0\Phi_{\text{Co,Fe,Mn}}$	A119	293823.2	0.0	-	-	-
$1\Phi_{\text{Co,Fe,Mn}}$	A120	0.0	264752.2	16339.1	178210.4	345302.4
$2\Phi_{\text{Co,Fe,Mn}}$	A121	0.0	0.0	-	-	-
$0\Phi_{\text{Co,Fe,Ni}}$	A122	-479480.0	0.0	-	-	-
$1\Phi_{\text{Co,Fe,Ni}}$	A123	0.0	0.0	-	-	-
$2\Phi_{\text{Co,Fe,Ni}}$	A124	0.0	198889.2	-128344.7	-80542.0	428650.8
$0\Phi_{\text{Co,Mn,Ni}}$	A125	273345.9	0.0	-	-	-
$1\Phi_{\text{Co,Mn,Ni}}$	A126	-323584.0	0.0	-	-	-
$2\Phi_{\text{Co,Mn,Ni}}$	A127	0.0	-316601.6	11505.1	-61206.1	-158715.5
$0\Phi_{\text{Cr,Fe,Mn}}$	A128	0.0	0.0	-	-	-
$1\Phi_{\text{Cr,Fe,Mn}}$	A129	176263.4	0.0	-	-	-
$2\Phi_{\text{Cr,Fe,Mn}}$	A130	0.0	0.0	-	-	-
$0\Phi_{\text{Cr,Fe,Ni}}$	A131	0.0	0.0	-	-	-
$1\Phi_{\text{Cr,Fe,Ni}}$	A132	0.0	0.0	-	-	-
$2\Phi_{\text{Cr,Fe,Ni}}$	A133	0.0	0.0	-	-	-
$0\Phi_{\text{Cr,Mn,Ni}}$	A134	-117266.8	0.0	-	-	-
$1\Phi_{\text{Cr,Mn,Ni}}$	A135	0.0	0.0	-	-	-
$2\Phi_{\text{Cr,Mn,Ni}}$	A136	241790.8	0.0	-	-	-
$0\Phi_{\text{Fe,Mn,Ni}}$	A137	99859.6	0.0	-	-	-
$1\Phi_{\text{Fe,Mn,Ni}}$	A138	0.0	-795300.3	3314.2	154913.3	-42763.1
$2\Phi_{\text{Fe,Mn,Ni}}$	A139	0.0	0.0	-	-	-
$0\Phi_{\text{Co,Cr,Fe}}$	A140	-610937.5	0.0	-	-	-
$1\Phi_{\text{Co,Cr,Fe}}$	A141	-685461.4	0.0	-	-	-
$2\Phi_{\text{Co,Cr,Fe}}$	A142	0.0	-150567.6	-266784.7	-358764.6	-1263059.7
$0\Phi_{\text{Co,Cr,Mn}}$	A143	0.0	-751055.9	-257049.6	-289679.0	-530645.2
$1\Phi_{\text{Co,Cr,Mn}}$	A144	-199578.9	-424292.0	-48852.5	-262622.1	-689742.4
$2\Phi_{\text{Co,Cr,Mn}}$	A145	0.0	0.0	-	-	-
$0\Phi_{\text{Co,Cr,Ni}}$	A146	-752667.2	-754278.6	56286.6	-68322.8	-873335.9

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Supplementary Table 2 – Lists of the parameters and their estimations (Continued)

Parameter	Notion	AIC	BIC	ReL1	ReL2	MCMC
$1\Phi_{\text{Mn}}^{\text{Co,Cr,Ni}}$	A147	0.0	0.0	-	-	-
$2\Phi_{\text{Mn}}^{\text{Co,Cr,Ni}}$	A148	0.0	254144.3	-135528.6	8215.3	-536826.5
$0\Phi_{\text{Mn}}^{\text{Co,Fe,Mn}}$	A149	-397503.7	0.0	-	-	-
$1\Phi_{\text{Mn}}^{\text{Co,Fe,Mn}}$	A150	0.0	0.0	-	-	-
$2\Phi_{\text{Mn}}^{\text{Co,Fe,Mn}}$	A151	-544940.2	0.0	-	-	-
$0\Phi_{\text{Mn}}^{\text{Co,Fe,Ni}}$	A152	137658.7	252264.4	277038.6	17950.4	184202.9
$1\Phi_{\text{Mn}}^{\text{Co,Fe,Ni}}$	A153	0.0	0.0	-	-	-
$2\Phi_{\text{Mn}}^{\text{Co,Fe,Ni}}$	A154	0.0	0.0	-	-	-
$0\Phi_{\text{Mn}}^{\text{Co,Mn,Ni}}$	A155	0.0	0.0	-	-	-
$1\Phi_{\text{Mn}}^{\text{Co,Mn,Ni}}$	A156	0.0	0.0	-	-	-
$2\Phi_{\text{Mn}}^{\text{Co,Mn,Ni}}$	A157	0.0	0.0	-	-	-
$0\Phi_{\text{Mn}}^{\text{Cr,Fe,Mn}}$	A158	-397772.2	0.0	-	-	-
$1\Phi_{\text{Mn}}^{\text{Cr,Fe,Mn}}$	A159	229168.7	0.0	-	-	-
$2\Phi_{\text{Mn}}^{\text{Cr,Fe,Mn}}$	A160	-408648.7	-603955.1	-311499.0	-135461.4	-41906.3
$0\Phi_{\text{Mn}}^{\text{Cr,Fe,Ni}}$	A161	-65704.3	0.0	-	-	-
$1\Phi_{\text{Mn}}^{\text{Cr,Fe,Ni}}$	A162	25402.8	0.0	-	-	-
$2\Phi_{\text{Mn}}^{\text{Cr,Fe,Ni}}$	A163	-485522.5	0.0	-	-	-
$0\Phi_{\text{Mn}}^{\text{Cr,Mn,Ni}}$	A164	0.0	0.0	-	-	-
$1\Phi_{\text{Mn}}^{\text{Cr,Mn,Ni}}$	A165	0.0	0.0	-	-	-
$2\Phi_{\text{Mn}}^{\text{Cr,Mn,Ni}}$	A166	-756427.0	0.0	-	-	-
$0\Phi_{\text{Mn}}^{\text{Fe,Mn,Ni}}$	A167	-264971.9	0.0	-	-	-
$1\Phi_{\text{Mn}}^{\text{Fe,Mn,Ni}}$	A168	0.0	-443829.3	115704.3	148132.3	1078837.1
$2\Phi_{\text{Mn}}^{\text{Fe,Mn,Ni}}$	A169	0.0	0.0	-	-	-
$0\Phi_{\text{Ni}}^{\text{Co,Cr,Fe}}$	A170	0.0	0.0	-	-	-
$1\Phi_{\text{Ni}}^{\text{Co,Cr,Fe}}$	A171	0.0	-340301.5	-266851.8	-330902.1	-1002745.3
$2\Phi_{\text{Ni}}^{\text{Co,Cr,Fe}}$	A172	0.0	0.0	-	-	-
$0\Phi_{\text{Ni}}^{\text{Co,Cr,Mn}}$	A173	0.0	0.0	-	-	-
$1\Phi_{\text{Ni}}^{\text{Co,Cr,Mn}}$	A174	-452557.4	0.0	-	-	-
$2\Phi_{\text{Ni}}^{\text{Co,Cr,Mn}}$	A175	0.0	0.0	-	-	-
$0\Phi_{\text{Ni}}^{\text{Co,Cr,Ni}}$	A176	68774.4	0.0	-	-	-
$1\Phi_{\text{Ni}}^{\text{Co,Cr,Ni}}$	A177	0.0	0.0	-	-	-
$2\Phi_{\text{Ni}}^{\text{Co,Cr,Ni}}$	A178	0.0	-503247.1	-332580.6	-271148.7	-1294090.5
$0\Phi_{\text{Ni}}^{\text{Co,Fe,Mn}}$	A179	0.0	0.0	-	-	-
$1\Phi_{\text{Ni}}^{\text{Co,Fe,Mn}}$	A180	0.0	0.0	-	-	-
$2\Phi_{\text{Ni}}^{\text{Co,Fe,Mn}}$	A181	0.0	0.0	-	-	-
$0\Phi_{\text{Ni}}^{\text{Co,Fe,Ni}}$	A182	0.0	0.0	-	-	-
$1\Phi_{\text{Ni}}^{\text{Co,Fe,Ni}}$	A183	0.0	0.0	-	-	-

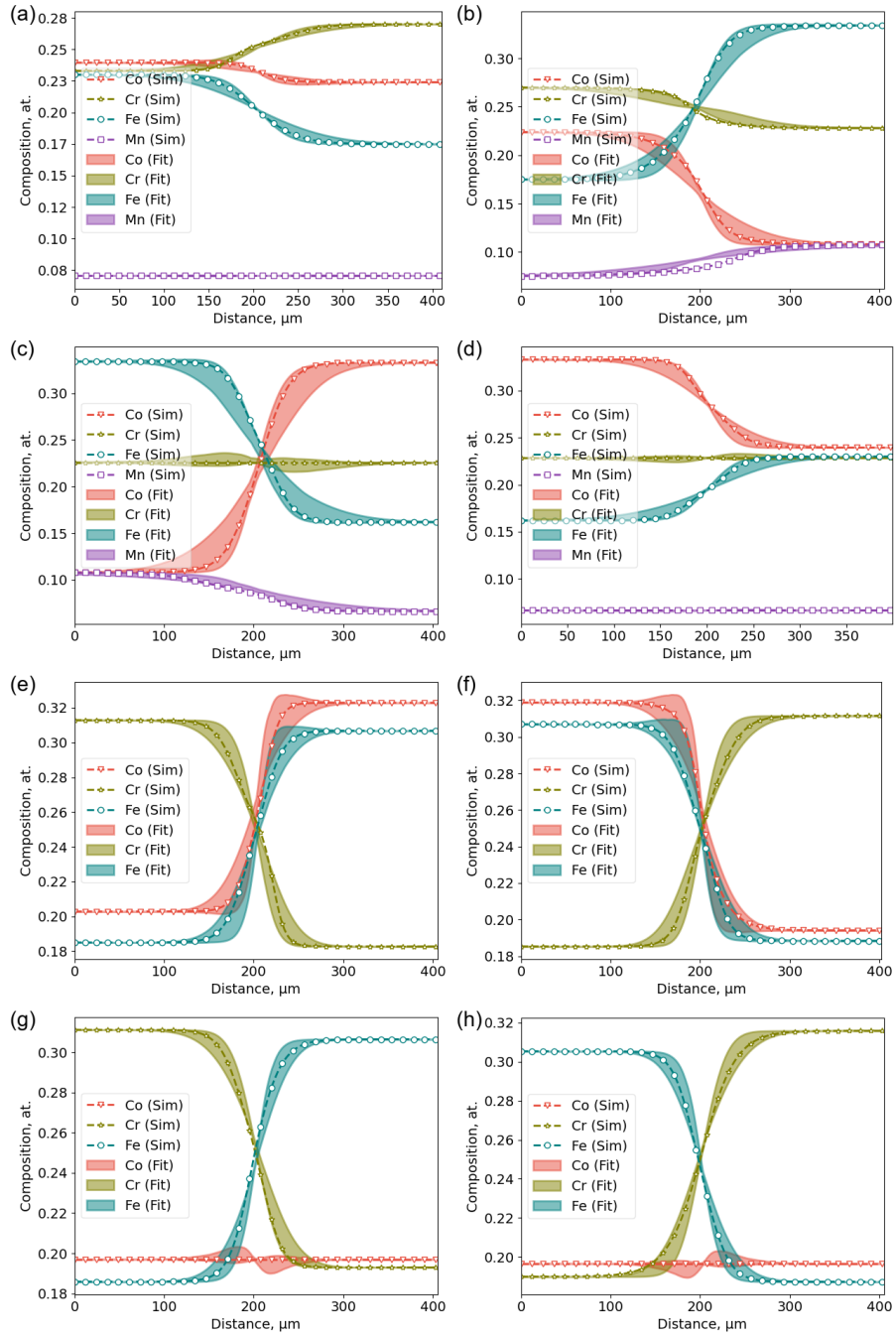
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Supplementary Table 2 – Lists of the parameters and their estimations (Continued)

Parameter	Notion	AIC	BIC	ReL1	ReL2	MCMC
$2\Phi_{\text{Ni}}^{\text{Co,Fe,Ni}}$	A184	0.0	0.0	-	-	-
$0\Phi_{\text{Ni}}^{\text{Co,Mn,Ni}}$	A185	0.0	0.0	-	-	-
$1\Phi_{\text{Ni}}^{\text{Co,Mn,Ni}}$	A186	34802.2	0.0	-	-	-
$2\Phi_{\text{Ni}}^{\text{Co,Mn,Ni}}$	A187	0.0	0.0	-	-	-
$0\Phi_{\text{Ni}}^{\text{Cr,Fe,Mn}}$	A188	0.0	0.0	-	-	-
$1\Phi_{\text{Ni}}^{\text{Cr,Fe,Mn}}$	A189	0.0	-339428.7	31042.5	-21392.8	-64798.4
$2\Phi_{\text{Ni}}^{\text{Cr,Fe,Mn}}$	A190	-566693.1	270660.4	-73693.8	-29919.4	297687.2
$0\Phi_{\text{Ni}}^{\text{Cr,Fe,Ni}}$	A191	0.0	0.0	-	-	-
$1\Phi_{\text{Ni}}^{\text{Cr,Fe,Ni}}$	A192	0.0	0.0	-	-	-
$2\Phi_{\text{Ni}}^{\text{Cr,Fe,Ni}}$	A193	0.0	0.0	-	-	-
$0\Phi_{\text{Ni}}^{\text{Cr,Mn,Ni}}$	A194	-518084.7	0.0	-	-	-
$1\Phi_{\text{Ni}}^{\text{Cr,Mn,Ni}}$	A195	-200585.9	0.0	-	-	-
$2\Phi_{\text{Ni}}^{\text{Cr,Mn,Ni}}$	A196	0.0	0.0	-	-	-
$0\Phi_{\text{Ni}}^{\text{Fe,Mn,Ni}}$	A197	-380450.4	0.0	-	-	-
$1\Phi_{\text{Ni}}^{\text{Fe,Mn,Ni}}$	A198	0.0	0.0	-	-	-
$2\Phi_{\text{Ni}}^{\text{Fe,Mn,Ni}}$	A199	-67651.4	0.0	-	-	-

Supplementary Table 3: Lists of the selected parameters and their estimations using diferent algorithms

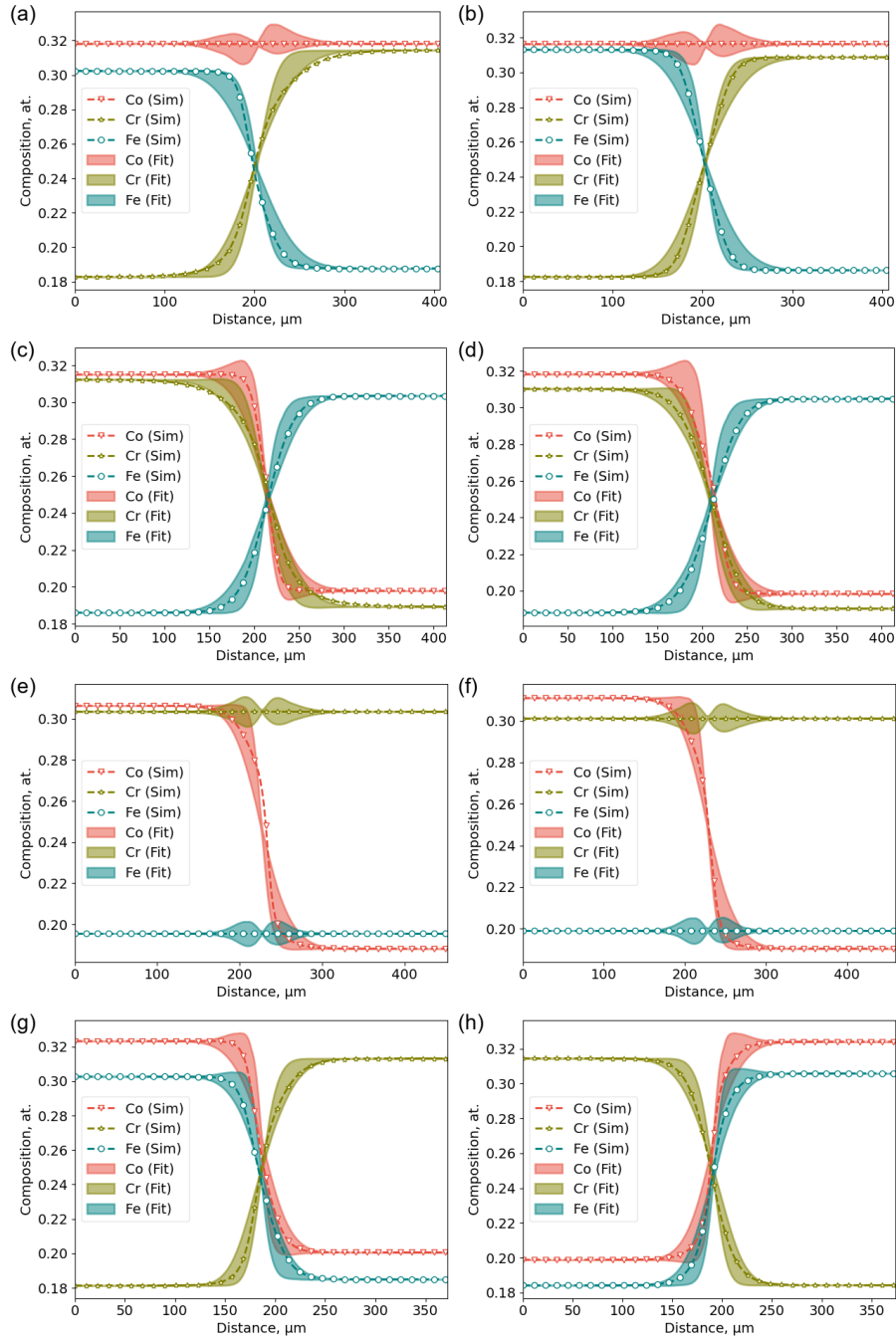
No.	Mobility Parameters	VarSelGA	L1 Re	L2 Re	Mean	MCMC Lower	Upper
1	$1\Phi_{Cr}^{Cr,Mn,Ni}$	-638330	32049	81127	-554963	-869979	-198537
2	$0\Phi_{Cr}^{Co,Fe}$	-175408	-127136	-132104	-119607	-155687	-83104
3	$2\Phi_{Fe}^{Co,Cr,Mn}$	-766430	-354400	48431	-308992	-757776	179089
4	$0\Phi_{Fe}^{Co,Cr,Ni}$	-611340	-189373	-41467	-1162293	-1499070	-837883
5	$1\Phi_{Fe}^{Co,Fe,Mn}$	264752	16339	178210	345302	62002	595788
6	$2\Phi_{Fe}^{Co,Fe,Ni}$	198889	-128344	-80541	428650	94625	762827
7	$2\Phi_{Fe}^{Co,Mn,Ni}$	-316601	11505	-61206	-158715	-562702	240798
8	$1\Phi_{Fe}^{Fe,Mn,Ni}$	-795300	3314	154913	-42763	-641325	455365
9	$2\Phi_{Mn}^{Co,Cr,Fe}$	-150567	-266784	-358764	-1263059	-1554740	-853629
10	$0\Phi_{Mn}^{Co,Cr,Mn}$	-751055	-257049	-289678	-530645	-1212457	-49678
11	$1\Phi_{Mn}^{Co,Cr,Mn}$	-424291	-48852	-262622	-689742	-1117400	-320052
12	$0\Phi_{Mn}^{Co,Cr,Ni}$	-754278	56286	-68322	-873335	-1154770	-609466
13	$2\Phi_{Mn}^{Co,Cr,Ni}$	254144	-135528	8215	-536826	-816154	-246228
14	$0\Phi_{Mn}^{Co,Fe,Ni}$	252264	277038	17950	184202	-109318	522592
15	$0\Phi_{Cr}^{Cr,Ni}$	-33612	-112164	-90008	-74623	-103839	-39300
16	$2\Phi_{Mn}^{Cr,Fe,Mn}$	-603955	-311499	-135461	-41906	-458187	421596
17	$1\Phi_{Mn}^{Fe,Mn,Ni}$	-443829	115704	148132	1078837	762541	1403700
18	$1\Phi_{Ni}^{Co,Cr,Fe}$	-340301	-266851	-330902	-1002745	-1570660	-484160
19	$2\Phi_{Ni}^{Co,Cr,Ni}$	-503247	-332580	-271148	-1294090	-1664110	-949025
20	$1\Phi_{Ni}^{Cr,Fe,Mn}$	-339428	31042	-21392	-64798	-511111	372495
21	$2\Phi_{Ni}^{Cr,Fe,Mn}$	270660	-73693	-29919	297687	-163241	726357
22	$0\Phi_{Co}^{Co,Mn}$	30572	26611	46618	-5065	-59532	48286
23	$0\Phi_{Fe}^{Cr,Fe}$	-163256	-176617	-220861	-159661	-187210	-131292
24	$0\Phi_{Fe}^{Mn,Ni}$	130877	105566	95294	67438	6374	130605
25	$0\Phi_{Mn}^{Co,Mn}$	293756	231384	256964	-5098	-39574	25478
26	$0\Phi_{Mn}^{Co,Ni}$	-254162	-252551	-250537	70728	33898	109891
27	$0\Phi_{Ni}^{Cr,Mn}$	-668475	-425500	-274304	-200146	-296114	-101756
28	$0\Phi_{Ni}^{Fe,Ni}$	-197631	-177893	-160906	-93045	-137759	-49203
29	$0\Phi_{Ni}^{Mn,Ni}$	261395	238098	122552	131669	84759	176788
30	$1\Phi_{Co}^{Co,Cr,Ni}$	-129016	-379510	-4473	-415332	-936208	132340
31	$0\Phi_{Co}^{Cr,Ni}$	-195349	-221801	-249664	-224317	-272512	-176121
32	$1\Phi_{Co}^{Co,Mn,Ni}$	-242547	-99676	118255	-480462	-1164928	169640
33	$1\Phi_{Co}^{Cr,Fe,Mn}$	-308544	31579	-29382	72237	-231854	361169
34	$1\Phi_{Cr}^{Co,Cr,Ni}$	-155938	217083	-263763	-320802	-694728	-64346
35	$2\Phi_{Cr}^{Co,Fe,Mn}$	-344262	-55566	39971	-533786	-828298	-223361
36	$0\Phi_{Cr}^{Co,Fe,Ni}$	109594	112078	164178	243389	-230097	692613



Supplementary Figure 10: Comparison between the experimental composition profiles (Fitted with preset functions) and the predicted composition profiles (Prediction using the optimized kinetic description): (a)-(d) [a1], (e)-(h) [a2]

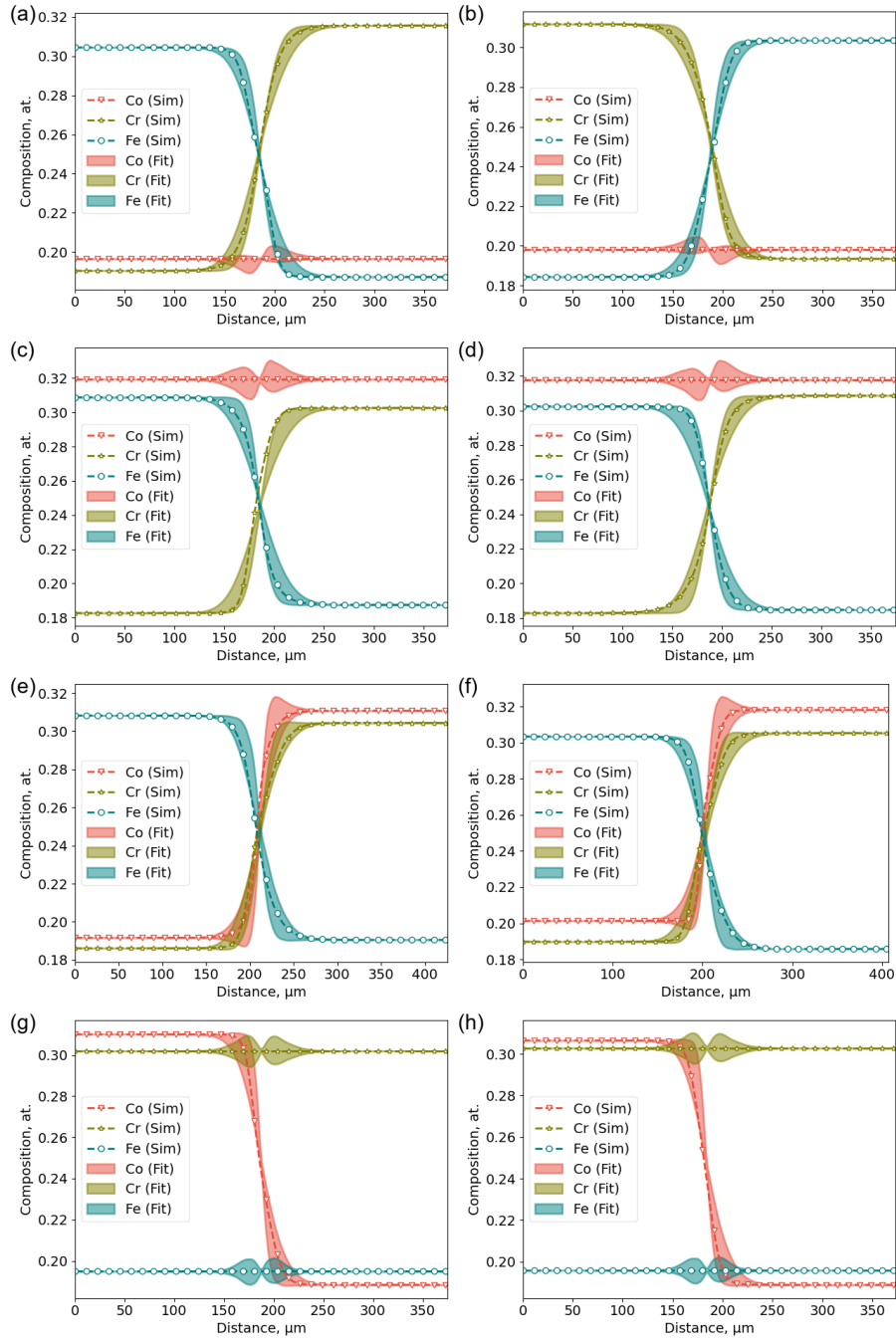
[a1] Chen, W. & Zhang, L. High-Throughput Determination of Interdiffusion Coefficients for Co-Cr-Fe-Mn-Ni High-Entropy Alloys. *J. Phase Equilib. Diffus.* 38, 457–465 (2017).

[a2] Dąbrowa, J. et al. Demystifying the sluggish diffusion effect in high entropy alloys. *J. Alloys Compd.* 783, 193–207 (2019).



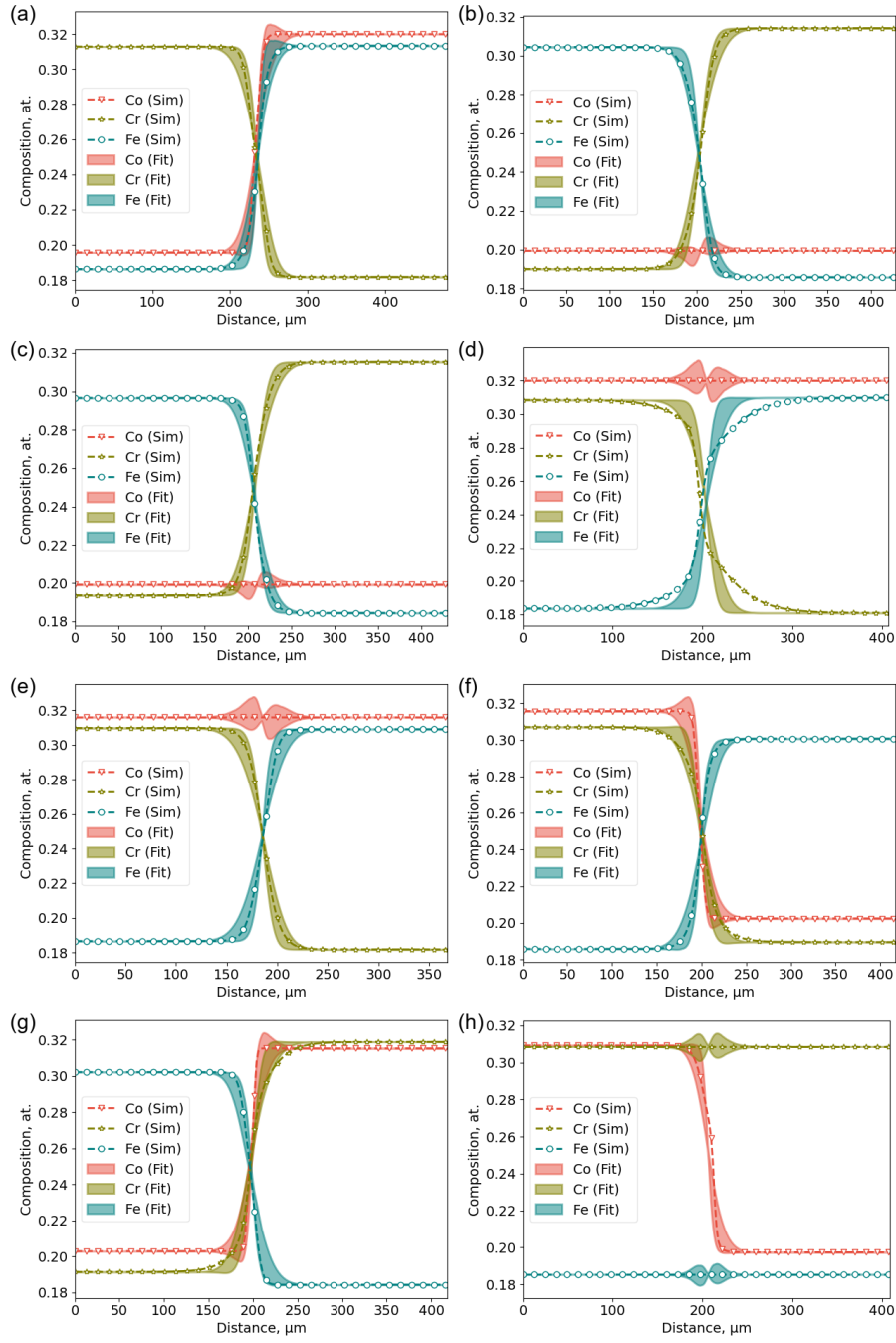
Supplementary Figure 11: Comparison between the experimental composition profiles (Fitted with preset functions) and the predicted composition profiles (Prediction using the optimized kinetic description): (a)-(h) [a3]

[a3] Dąbrowa, J. et al. Demystifying the sluggish diffusion effect in high entropy alloys. *J. Alloys Compd.* 783, 193–207 (2019).



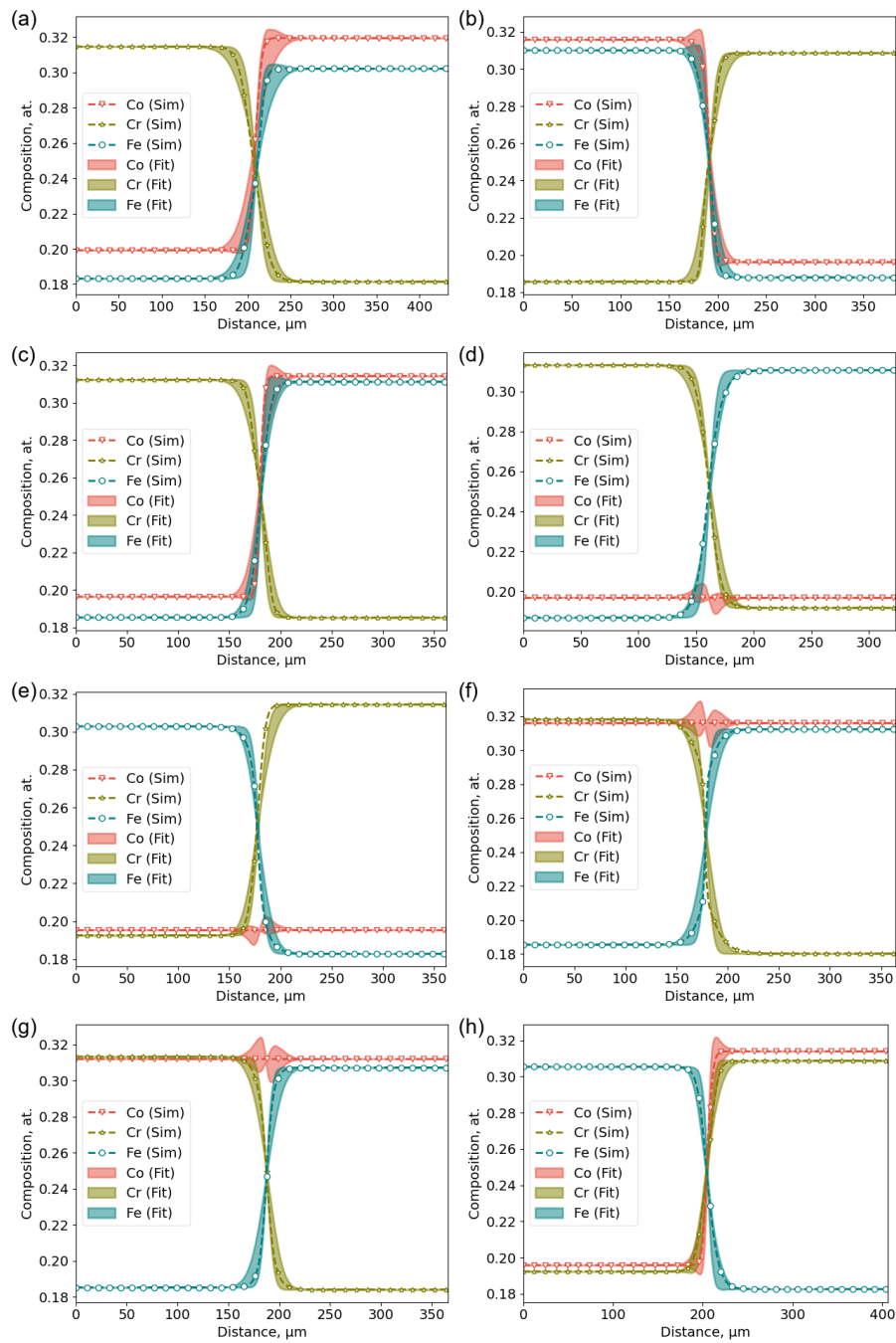
Supplementary Figure 12: Comparison between the experimental composition profiles (Fitted with preset functions) and the predicted composition profiles (Prediction using the optimized kinetic description): (a)-(h) [a4]

[a4] Dąbrowa, J. et al. Demystifying the sluggish diffusion effect in high entropy alloys. *J. Alloys Compd.* 783, 193–207 (2019).



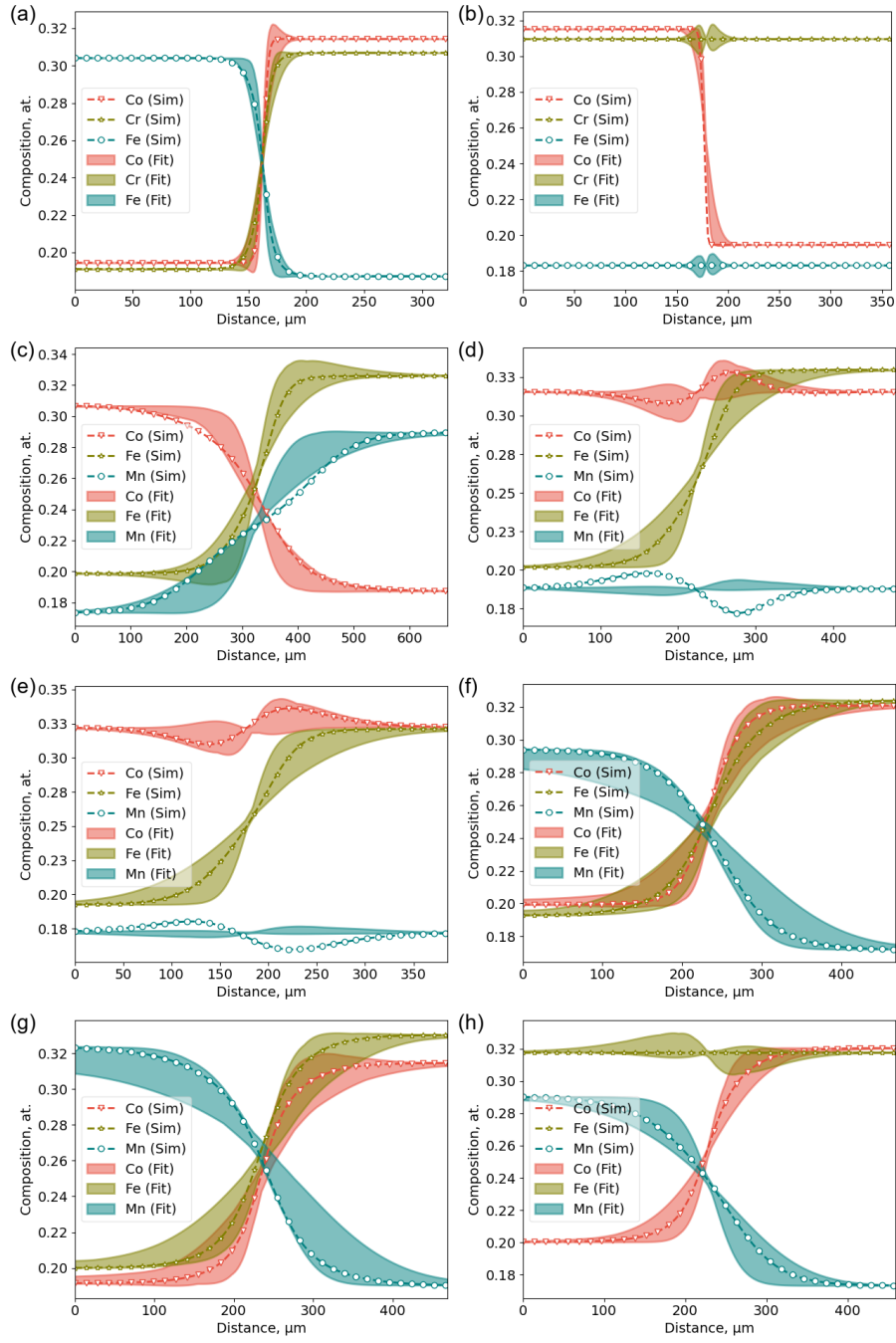
Supplementary Figure 13: Comparison between the experimental composition profiles (Fitted with preset functions) and the predicted composition profiles (Prediction using the optimized kinetic description): (a)-(h) [a5]

[a5] Dąbrowa, J. et al. Demystifying the sluggish diffusion effect in high entropy alloys. *J. Alloys Compd.* 783, 193–207 (2019).



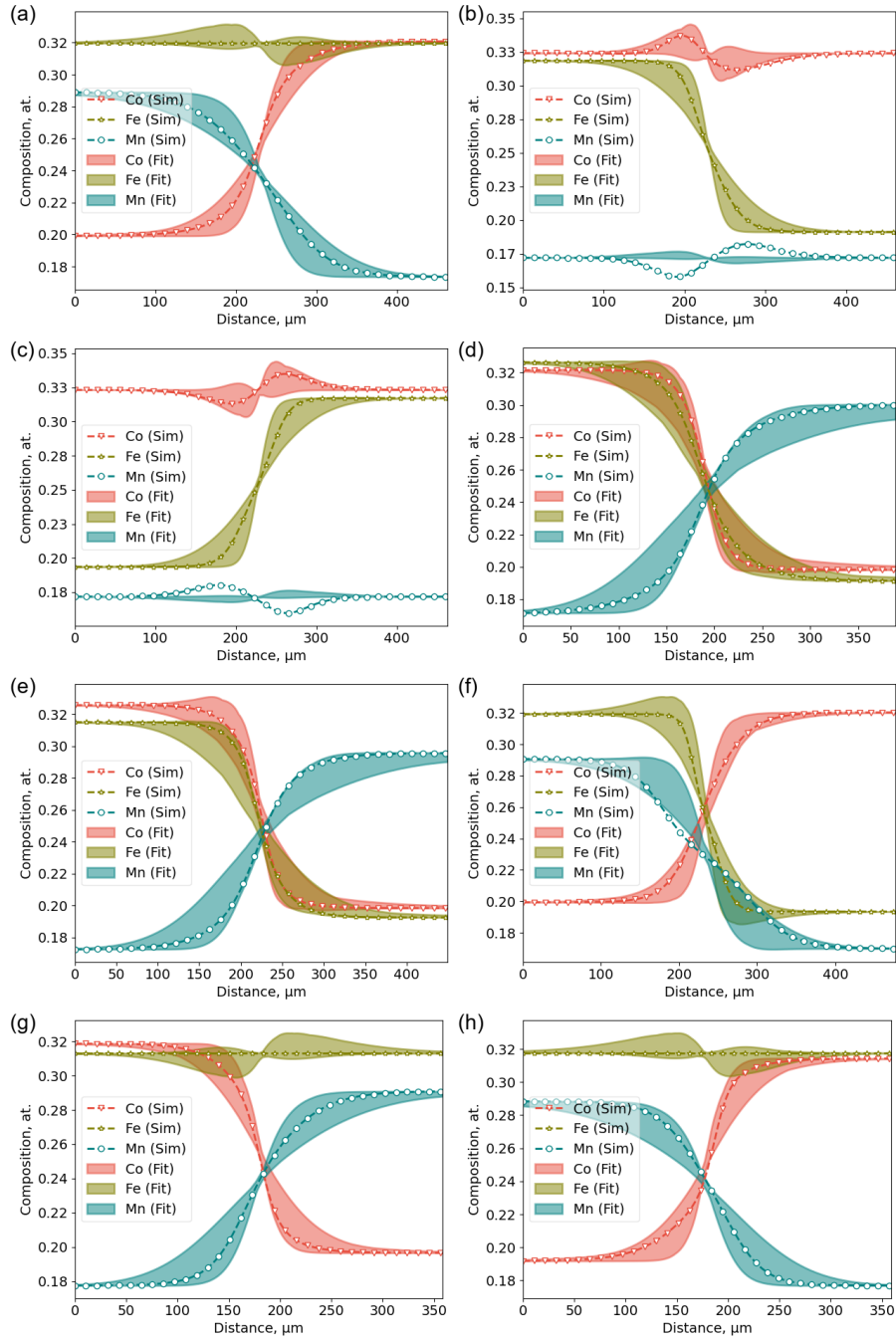
Supplementary Figure 14: Comparison between the experimental composition profiles (Fitted with preset functions) and the predicted composition profiles (Prediction using the optimized kinetic description): (a)-(h) [a6]

[a6] Dąbrowa, J. et al. Demystifying the sluggish diffusion effect in high entropy alloys. *J. Alloys Compd.* 783, 193–207 (2019).



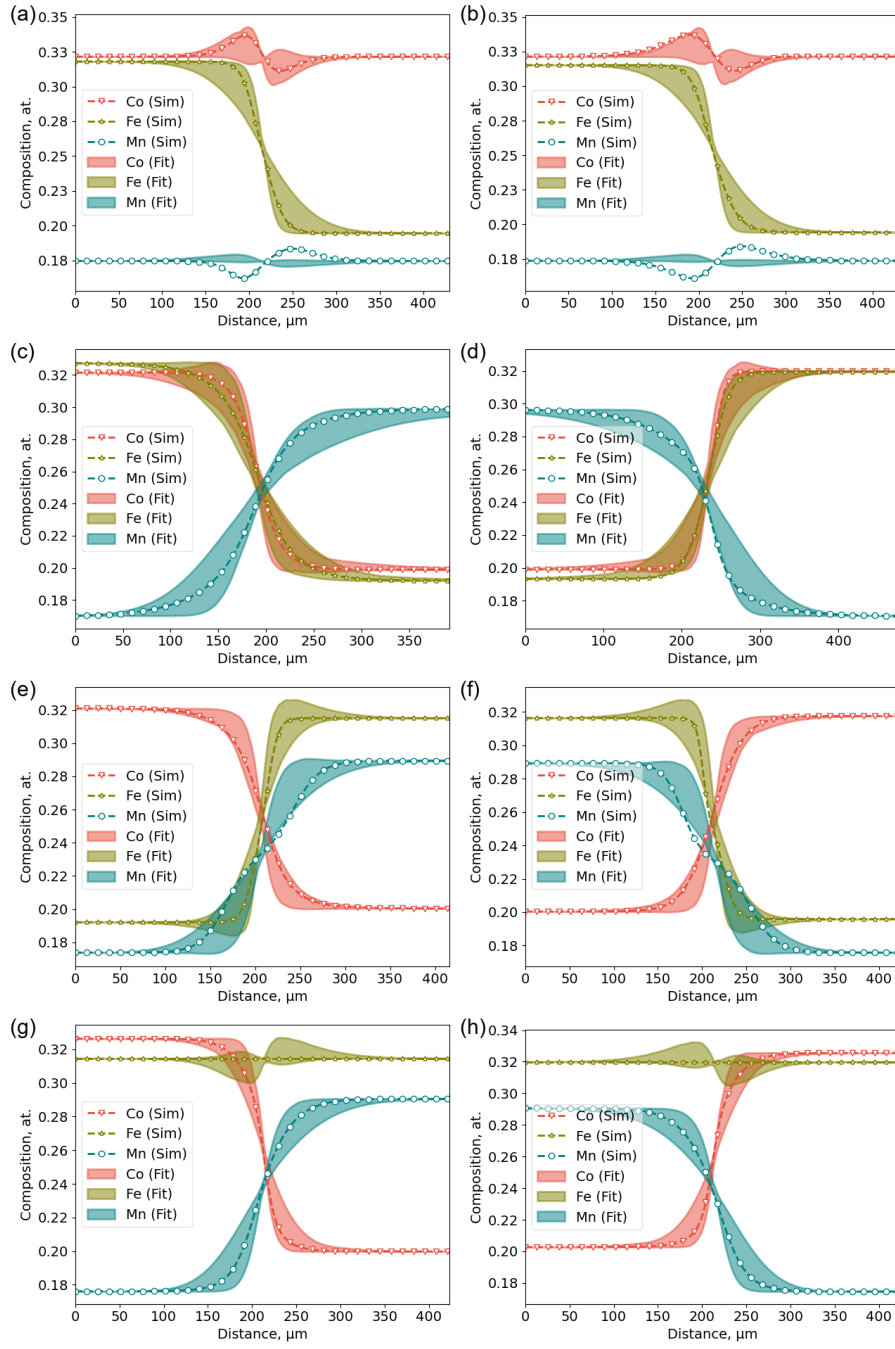
Supplementary Figure 15: Comparison between the experimental composition profiles (Fitted with preset functions) and the predicted composition profiles (Prediction using the optimized kinetic description): (a)-(h) [a7]

[a7] Dąbrowa, J. et al. Demystifying the sluggish diffusion effect in high entropy alloys. *J. Alloys Compd.* 783, 193–207 (2019).



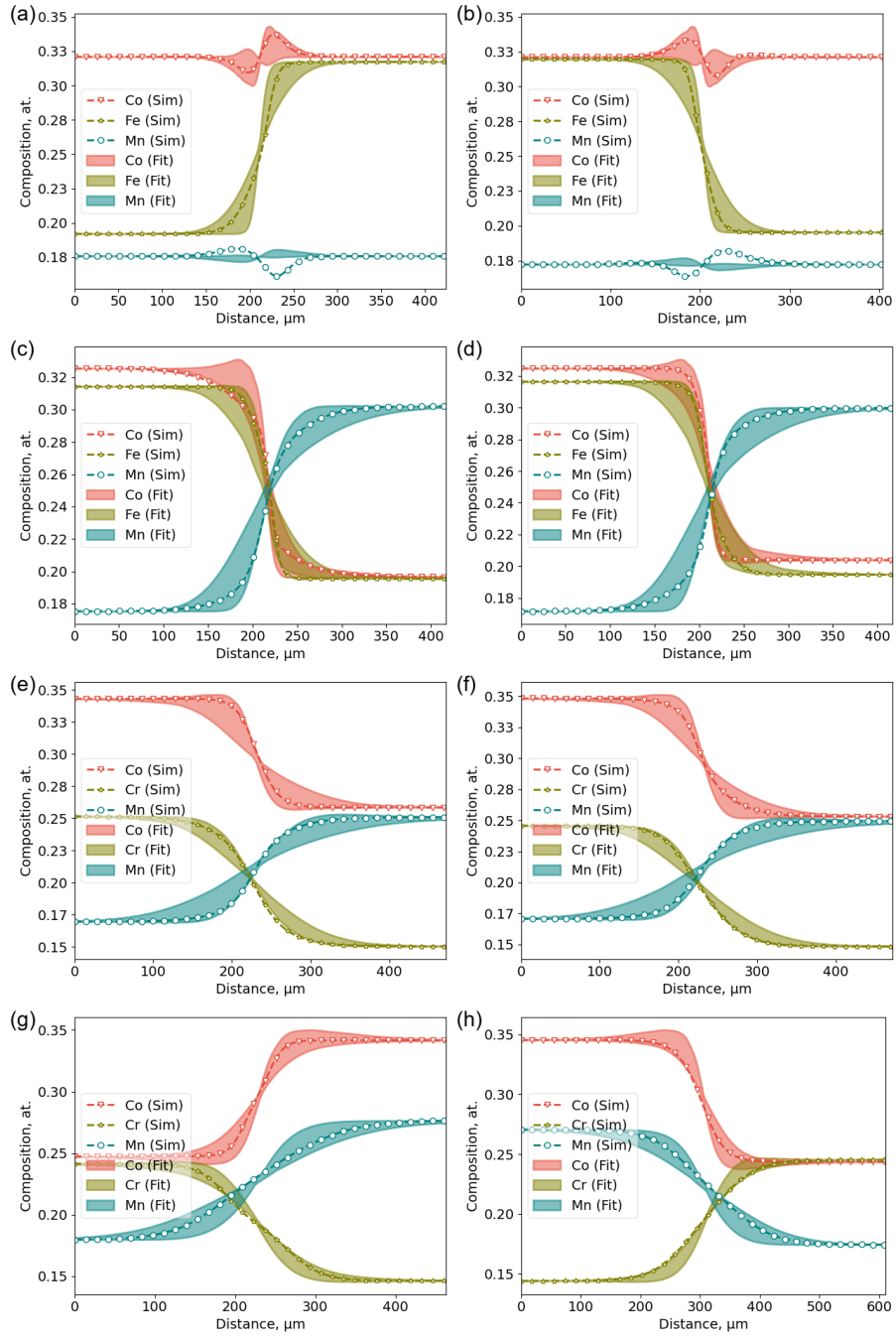
Supplementary Figure 16: Comparison between the experimental composition profiles (Fitted with preset functions) and the predicted composition profiles (Prediction using the optimized kinetic description): (a)-(h) [a8]

[a8] Dąbrowa, J. et al. Demystifying the sluggish diffusion effect in high entropy alloys. *J. Alloys Compd.* 783, 193–207 (2019).



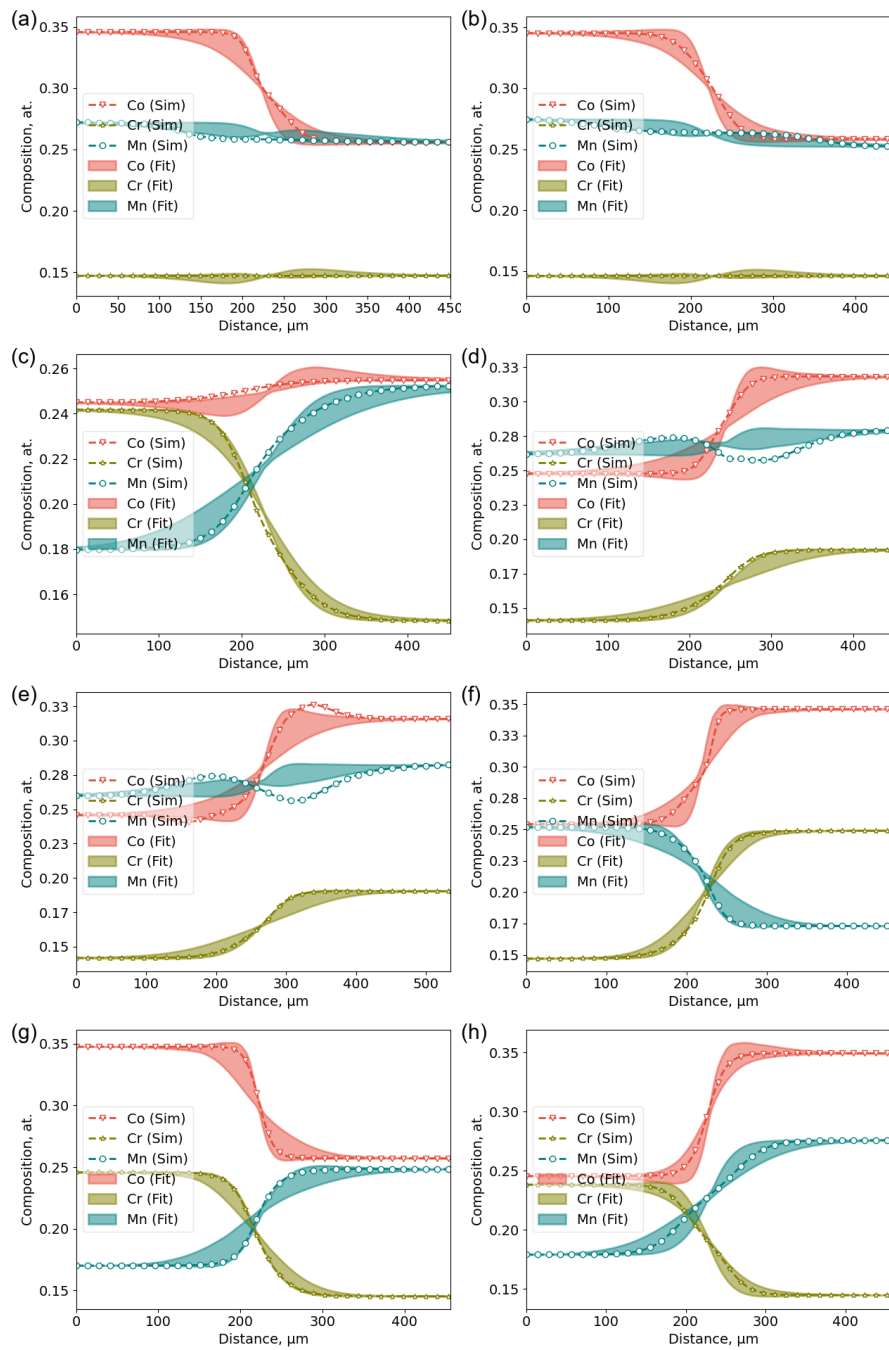
Supplementary Figure 17: Comparison between the experimental composition profiles (Fitted with preset functions) and the predicted composition profiles (Prediction using the optimized kinetic description): (a)-(h) [a9]

[a9] Dąbrowa, J. et al. Demystifying the sluggish diffusion effect in high entropy alloys. *J. Alloys Compd.* 783, 193–207 (2019).



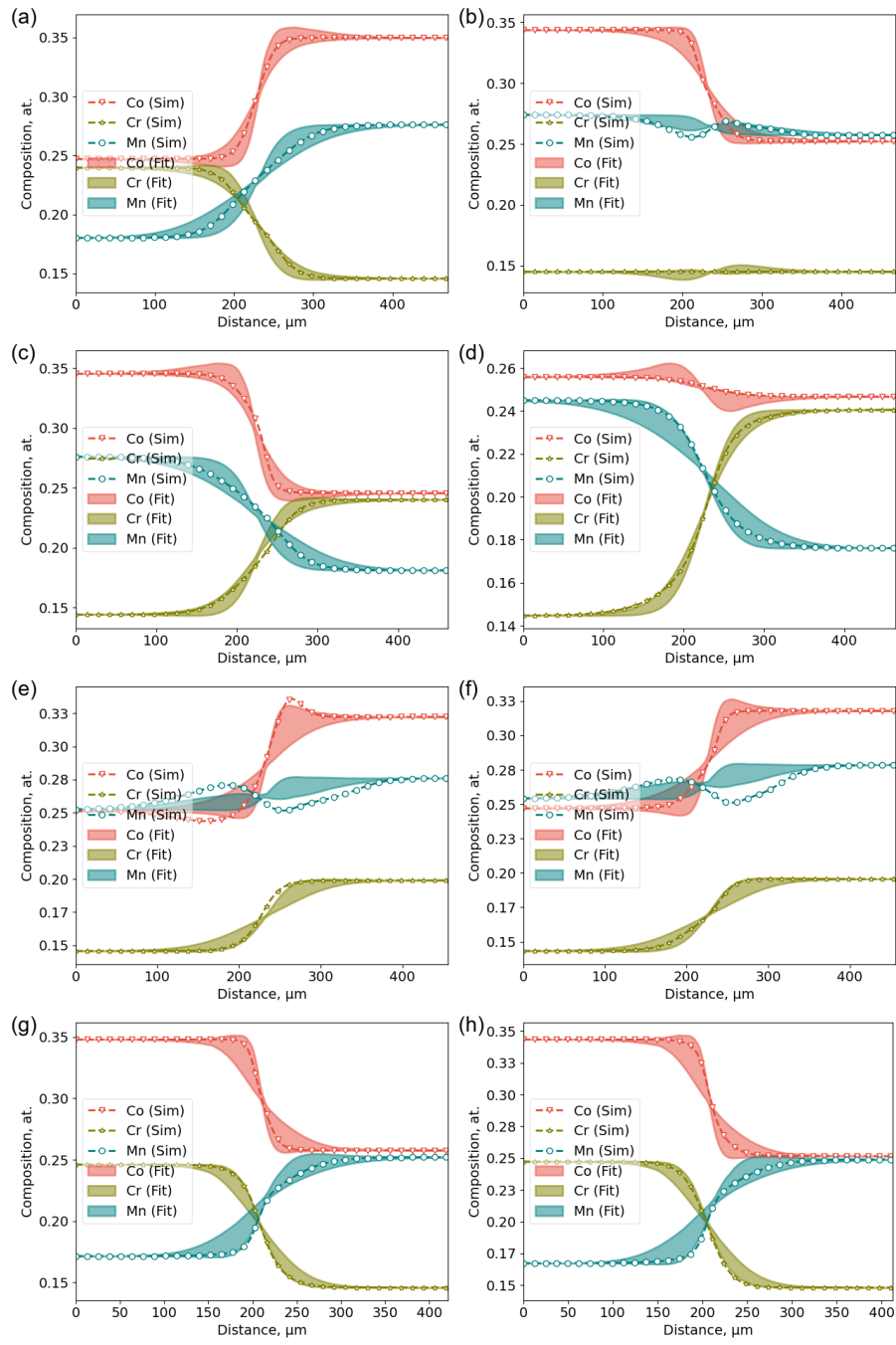
Supplementary Figure 18: Comparison between the experimental composition profiles (Fitted with preset functions) and the predicted composition profiles (Prediction using the optimized kinetic description): (a)-(h) [a10]

[a10] Dąbrowa, J. et al. Demystifying the sluggish diffusion effect in high entropy alloys. *J. Alloys Compd.* 783, 193–207 (2019).



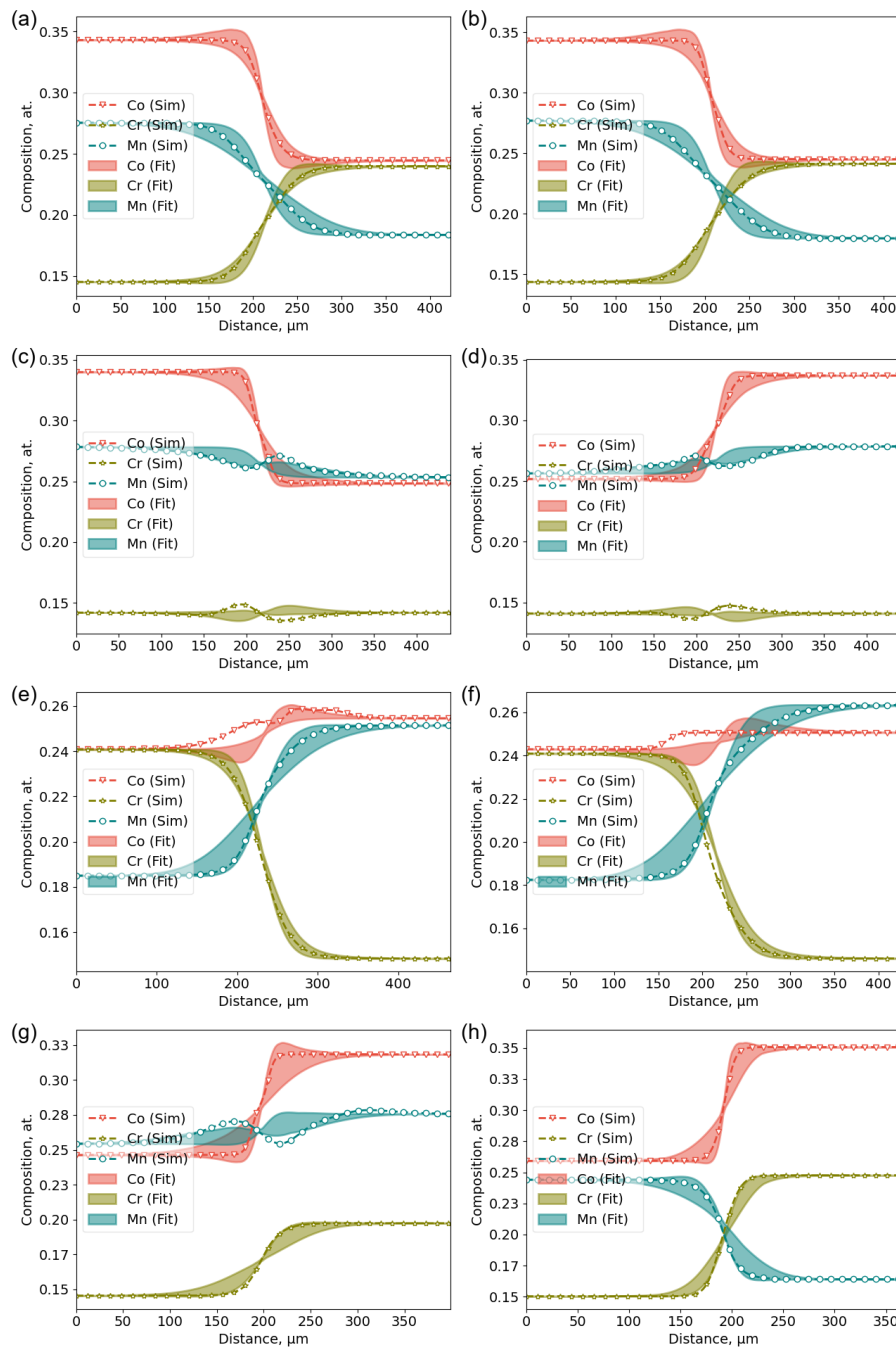
Supplementary Figure 19: Comparison between the experimental composition profiles (Fitted with preset functions) and the predicted composition profiles (Prediction using the optimized kinetic description): (a)-(h) [a11]

[a11] Dąbrowa, J. et al. Demystifying the sluggish diffusion effect in high entropy alloys. J. Alloys Compd. 783, 193–207 (2019).



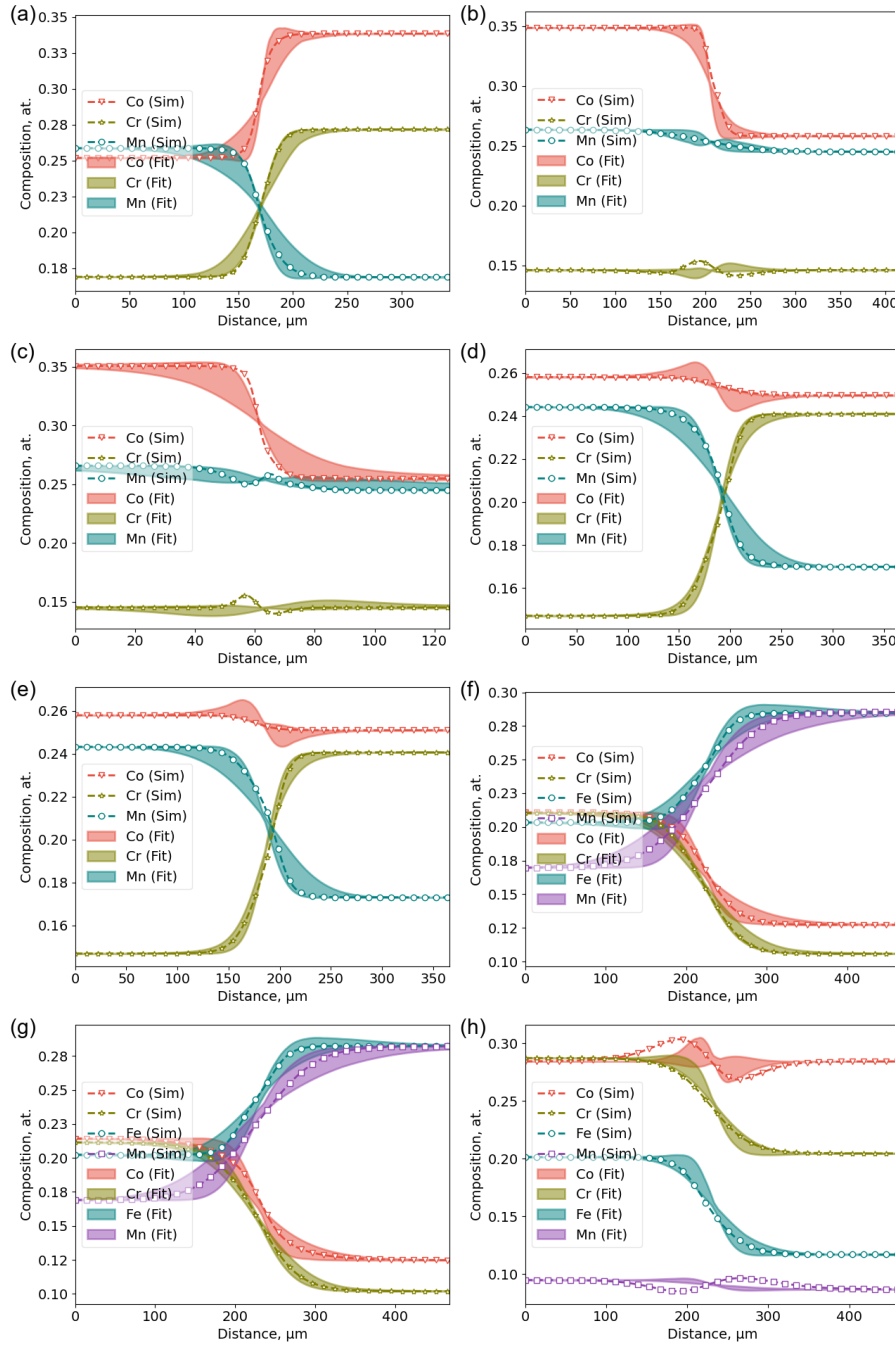
Supplementary Figure 20: Comparison between the experimental composition profiles (Fitted with preset functions) and the predicted composition profiles (Prediction using the optimized kinetic description): (a)-(h) [a12]

[a12] Dąbrowa, J. et al. Demystifying the sluggish diffusion effect in high entropy alloys. *J. Alloys Compd.* 783, 193–207 (2019).



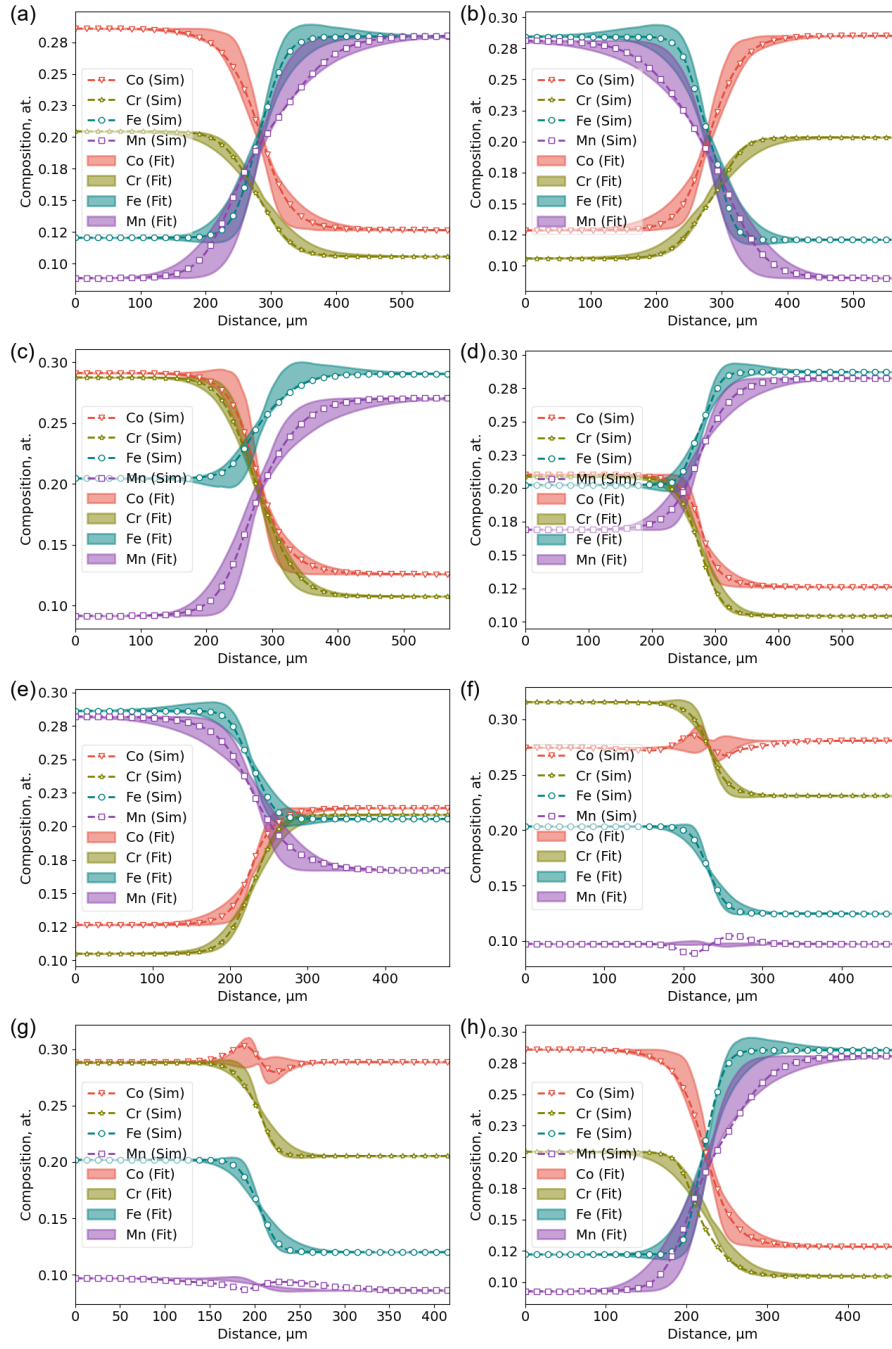
Supplementary Figure 21: Comparison between the experimental composition profiles (Fitted with preset functions) and the predicted composition profiles (Prediction using the optimized kinetic description): (a)-(h) [a13]

[a13] Dąbrowa, J. et al. Demystifying the sluggish diffusion effect in high entropy alloys. *J. Alloys Compd.* 783, 193–207 (2019).



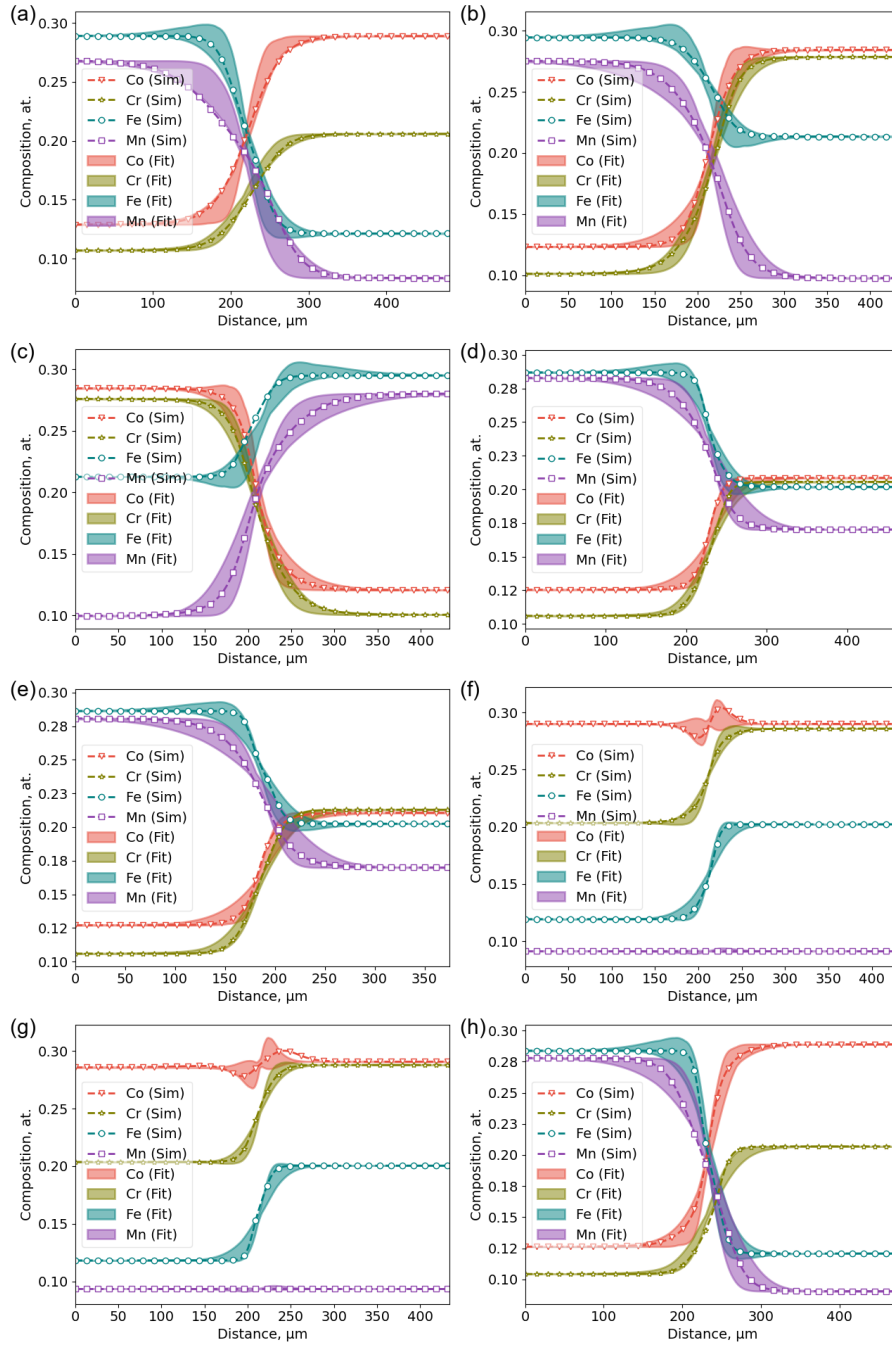
Supplementary Figure 22: Comparison between the experimental composition profiles (Fitted with preset functions) and the predicted composition profiles (Prediction using the optimized kinetic description): (a)-(h) [a14]

[a14] Dąbrowa, J. et al. Demystifying the sluggish diffusion effect in high entropy alloys. *J. Alloys Compd.* 783, 193–207 (2019).



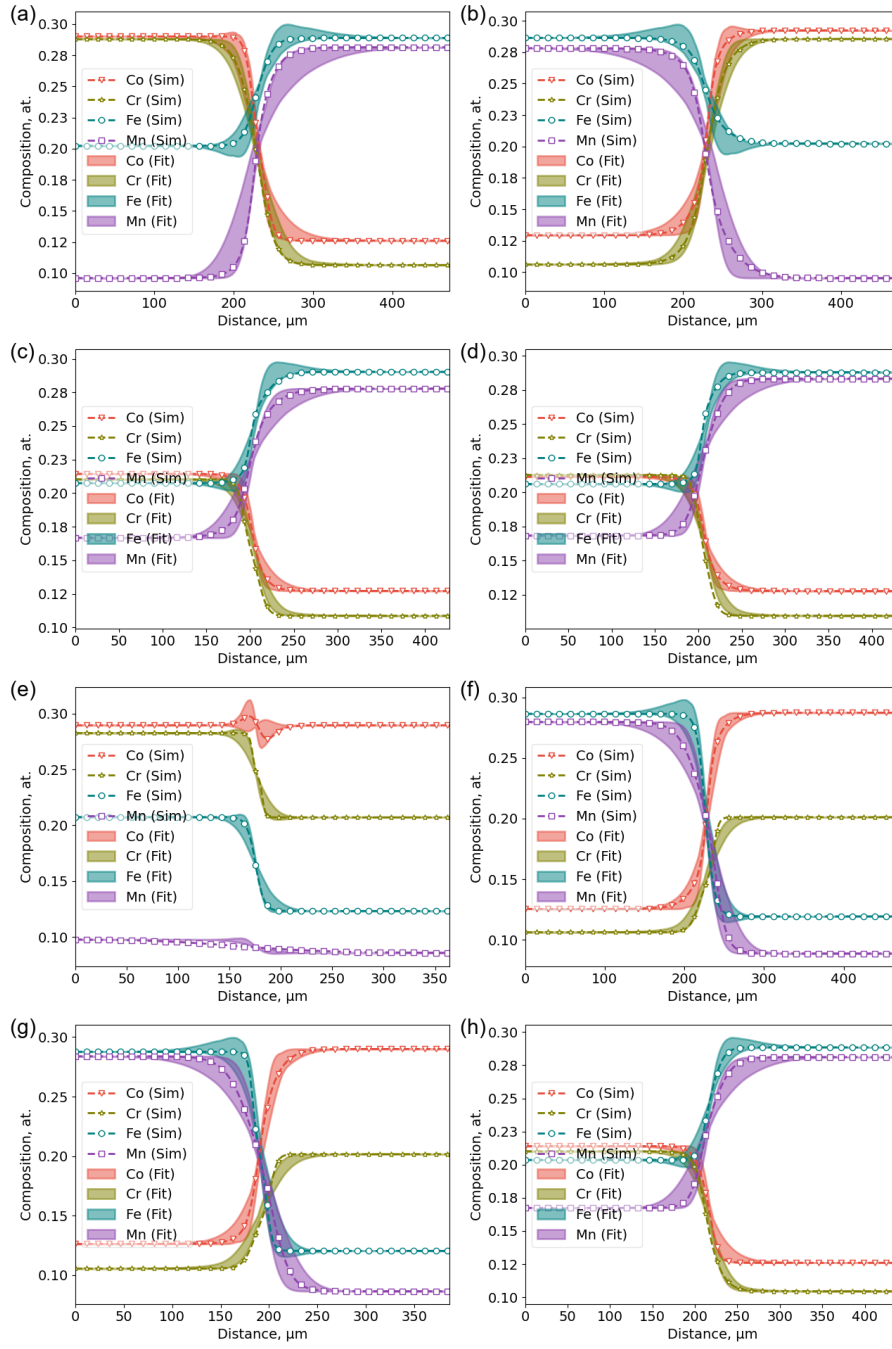
Supplementary Figure 23: Comparison between the experimental composition profiles (Fitted with preset functions) and the predicted composition profiles (Prediction using the optimized kinetic description): (a)-(h) [a15]

[a15] Dąbrowa, J. et al. Demystifying the sluggish diffusion effect in high entropy alloys. *J. Alloys Compd.* 783, 193–207 (2019).



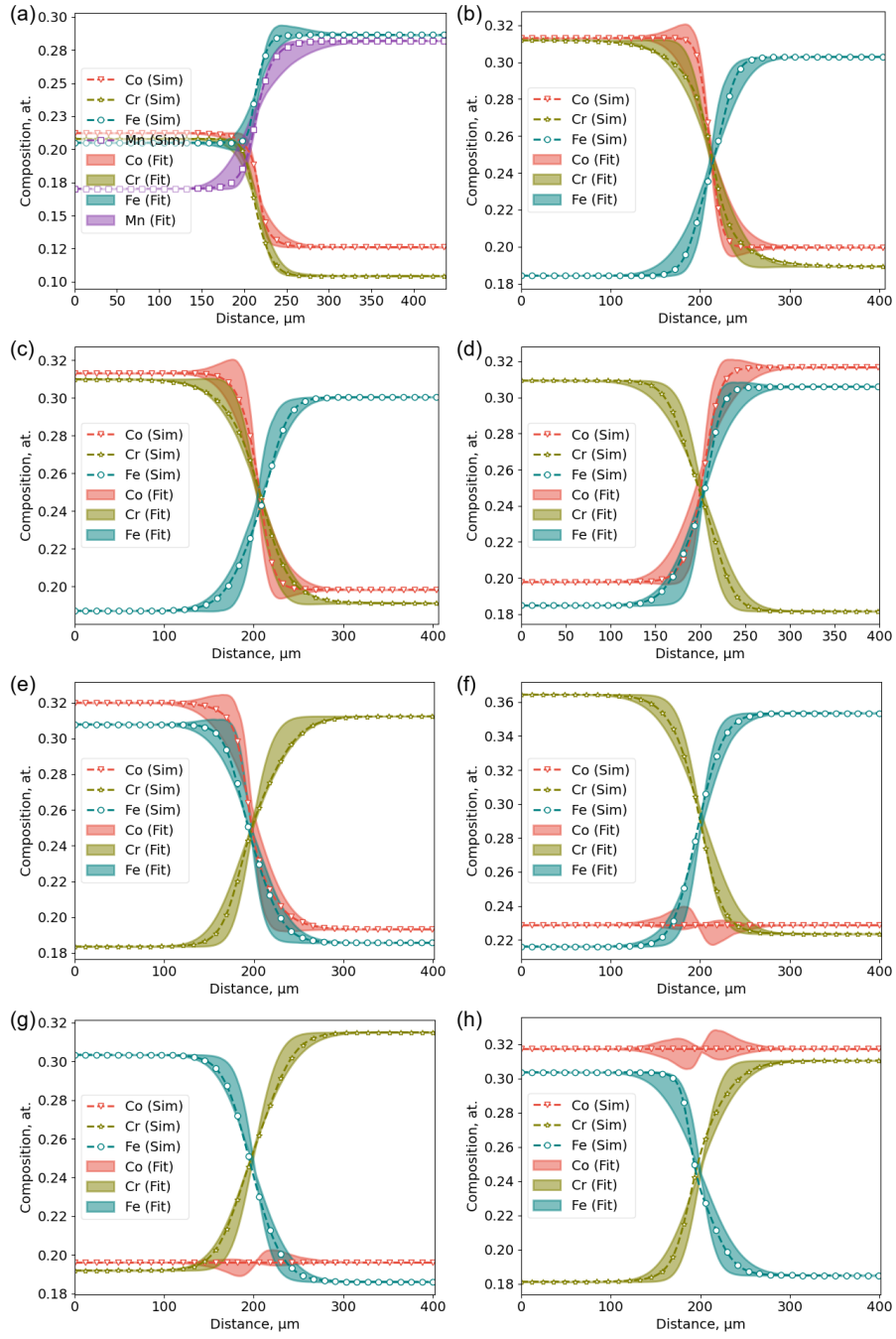
Supplementary Figure 24: Comparison between the experimental composition profiles (Fitted with preset functions) and the predicted composition profiles (Prediction using the optimized kinetic description): (a)-(h) [a16]

[a16] Dąbrowa, J. et al. Demystifying the sluggish diffusion effect in high entropy alloys. *J. Alloys Compd.* 783, 193–207 (2019).



Supplementary Figure 25: Comparison between the experimental composition profiles (Fitted with preset functions) and the predicted composition profiles (Prediction using the optimized kinetic description): (a)-(h) [a17]

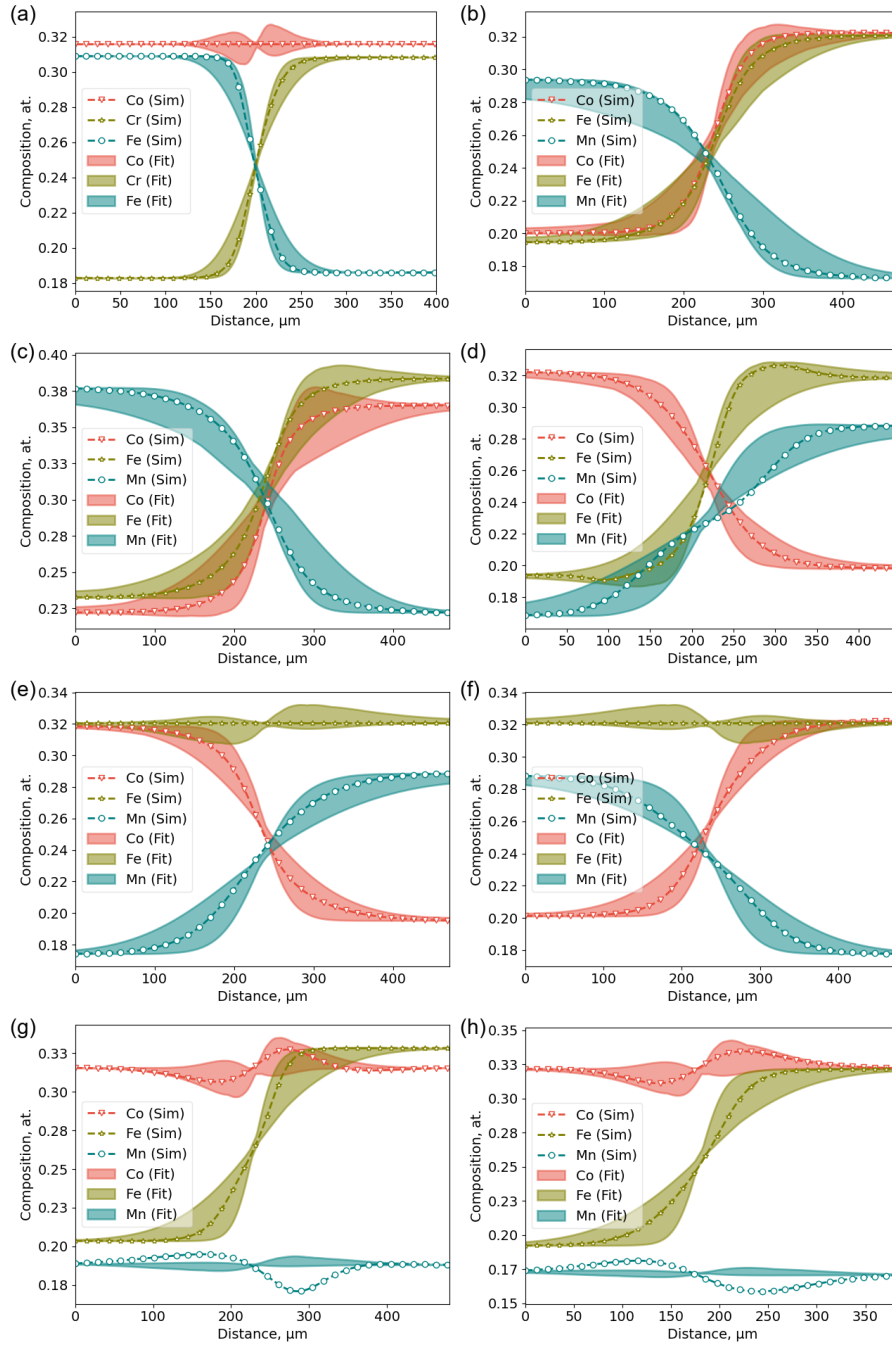
[a17] Dąbrowa, J. et al. Demystifying the sluggish diffusion effect in high entropy alloys. *J. Alloys Compd.* 783, 193–207 (2019).



Supplementary Figure 26: Comparison between the experimental composition profiles (Fitted with preset functions) and the predicted composition profiles (Prediction using the optimized kinetic description): (a) [a18], (b)-(h) [a19]

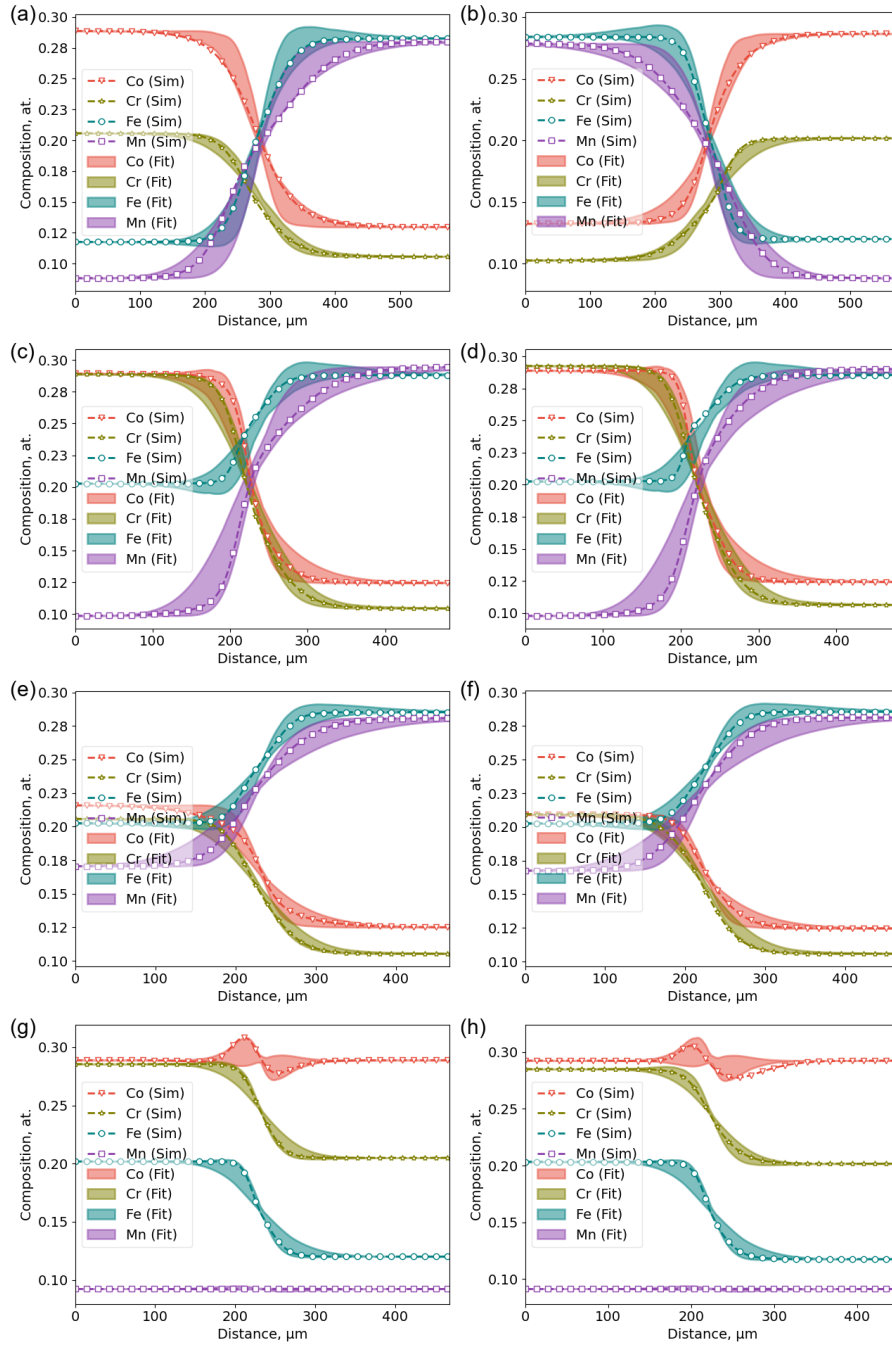
[a18] Dąbrowa, J. et al. Demystifying the sluggish diffusion effect in high entropy alloys. *J. Alloys Compd.* 783, 193–207 (2019).

[a19] Kucza, W. et al. Studies of “sluggish diffusion” effect in Co-Cr-Fe-Mn-Ni, Co-Cr-Fe-Ni and Co-Fe-Mn-Ni high entropy alloys; determination of tracer diffusivities by combinatorial approach. *J. Alloys Compd.* 731, 920–928 (2018).



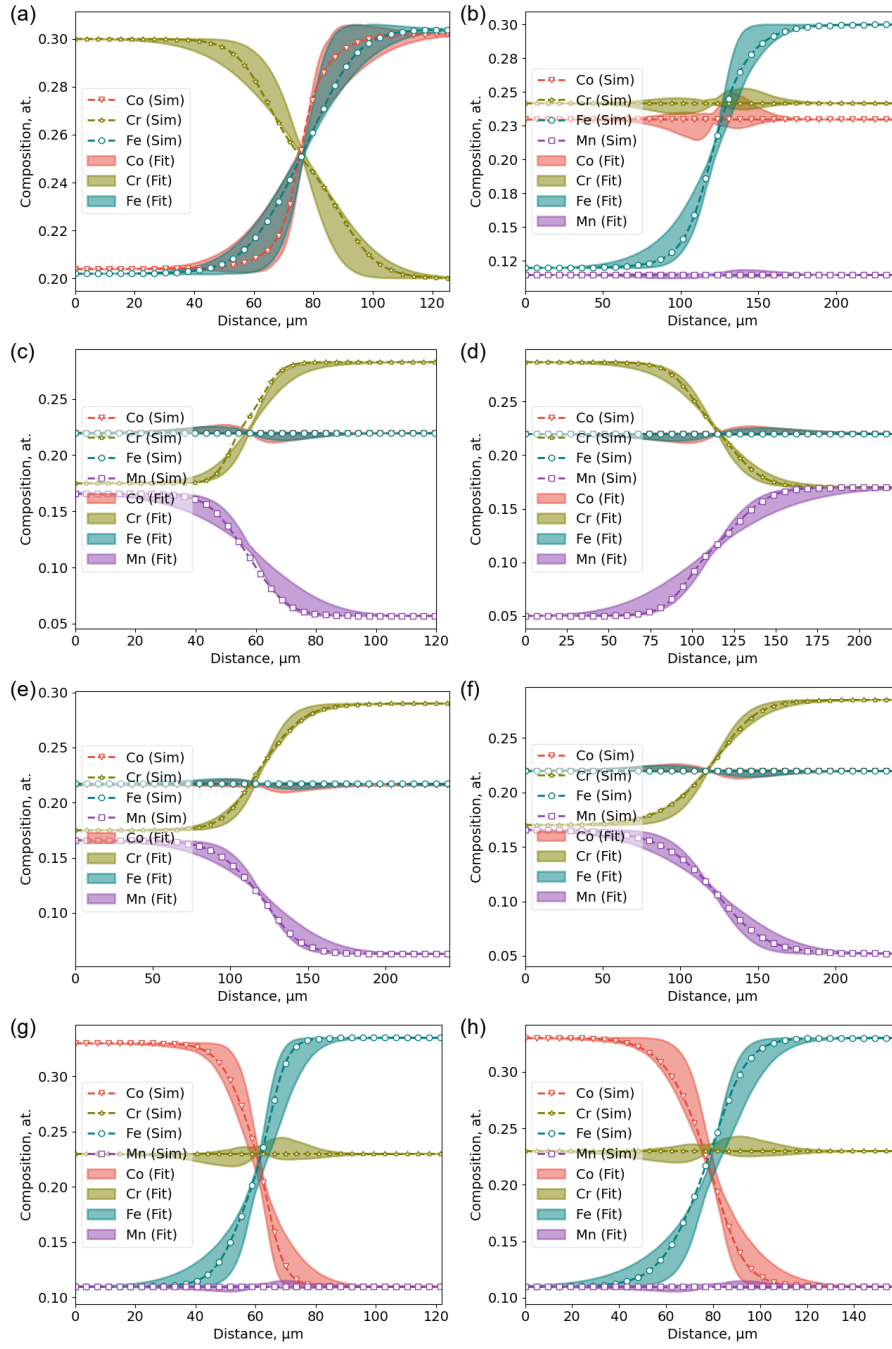
Supplementary Figure 27: Comparison between the experimental composition profiles (Fitted with preset functions) and the predicted composition profiles (Prediction using the optimized kinetic description): (a)-(h) [a20]

[a20] Kucza, W. et al. Studies of “sluggish diffusion” effect in Co-Cr-Fe-Mn-Ni, Co-Cr-Fe-Ni and Co-Fe-Mn-Ni high entropy alloys; determination of tracer diffusivities by combinatorial approach. J. Alloys Compd. 731, 920–928 (2018).



Supplementary Figure 28: Comparison between the experimental composition profiles (Fitted with preset functions) and the predicted composition profiles (Prediction using the optimized kinetic description): (a)-(h) [a21]

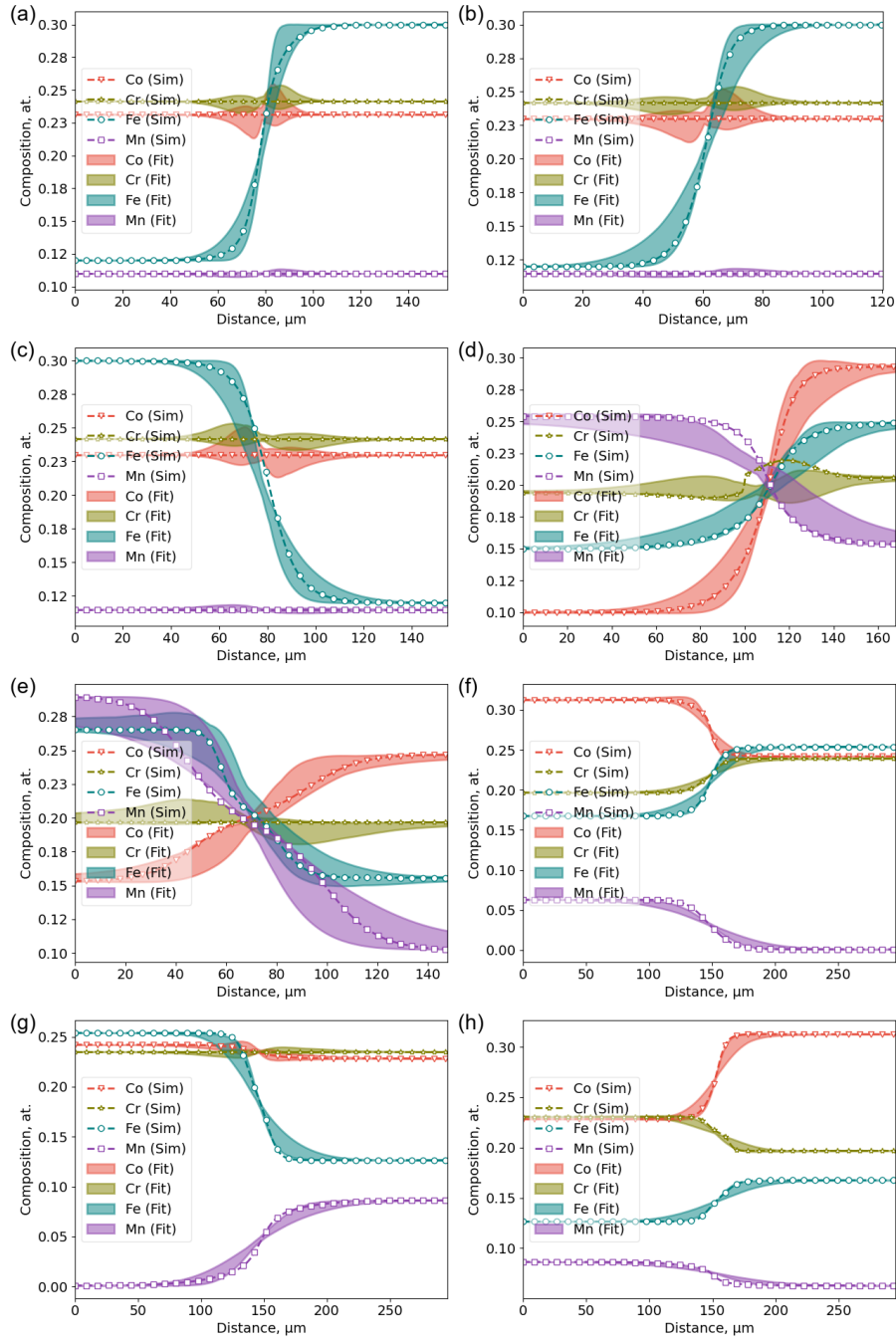
[a21] Kucza, W. et al. Studies of “sluggish diffusion” effect in Co-Cr-Fe-Mn-Ni, Co-Cr-Fe-Ni and Co-Fe-Mn-Ni high entropy alloys; determination of tracer diffusivities by combinatorial approach. *J. Alloys Compd.* 731, 920–928 (2018).



Supplementary Figure 29: Comparison between the experimental composition profiles (Fitted with preset functions) and the predicted composition profiles (Prediction using the optimized kinetic description): (a) [a22], (b)-(h) [a23]

[a22] Kulkarni, K. & Chauhan, G. P. S. Investigations of quaternary interdiffusion in a constituent system of high entropy alloys. AIP Advances 5, 097162 (2015).

[a23] Tsai, K.-Y., Tsai, M.-H. & Yeh, J.-W. Sluggish diffusion in Co–Cr–Fe–Mn–Ni high-entropy alloys. Acta Mater. 61, 4887–4897 (2013).

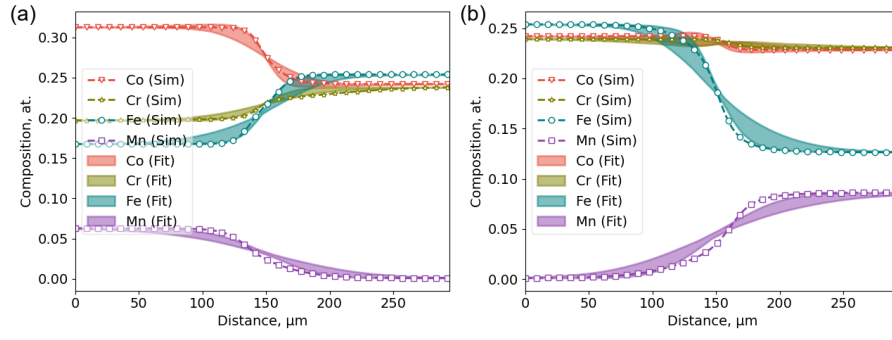


Supplementary Figure 30: Comparison between the experimental composition profiles (Fitted with preset functions) and the predicted composition profiles (Prediction using the optimized kinetic description): (a)-(c) [a24], (d)-(e) [a25], (f)-(h) [a26]

[a24] Tsai, K.-Y., Tsai, M.-H. & Yeh, J.-W. Sluggish diffusion in Co–Cr–Fe–Mn–Ni high-entropy alloys. *Acta Mater.* 61, 4887–4897 (2013).

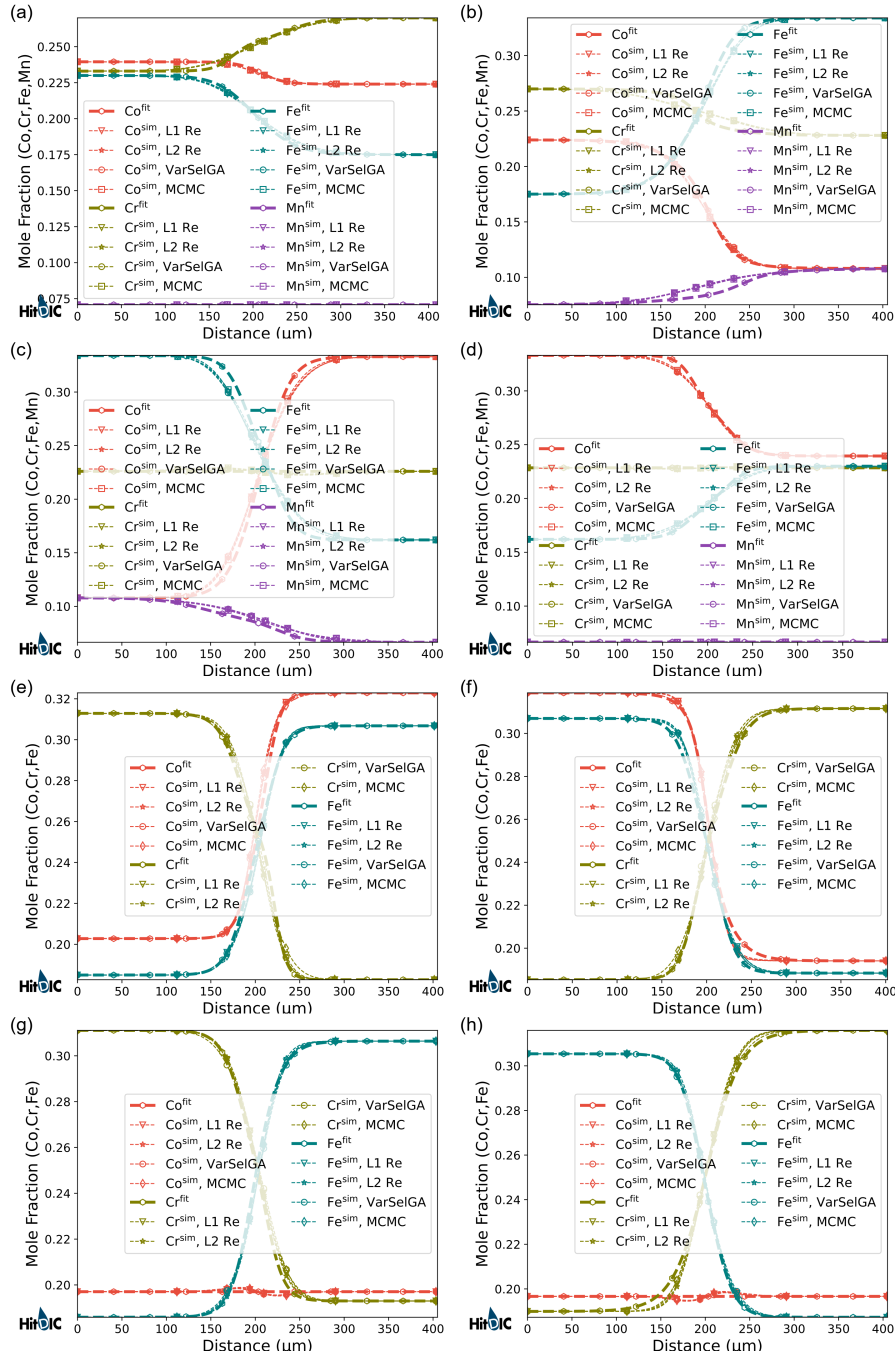
[a25] Verma, V., Tripathi, A. & Kulkarni, K. N. On Interdiffusion in FeNiCoCrMn High Entropy Alloy. *J. Phase Equilib. Diffus.* 38, 445–456 (2017).

[a26] R. Wang, On the determination of diffusion coefficients and sluggish diffusion effect of face-centered cubic Co–Cr–Fe–Ni–X(X=Mn,Cu) high entropy alloys, Master thesis (2018).



Supplementary Figure 31: Comparison between the experimental composition profiles (Fitted with preset functions) and the predicted composition profiles (Prediction using the optimized kinetic description): (a)-(b) [a27]

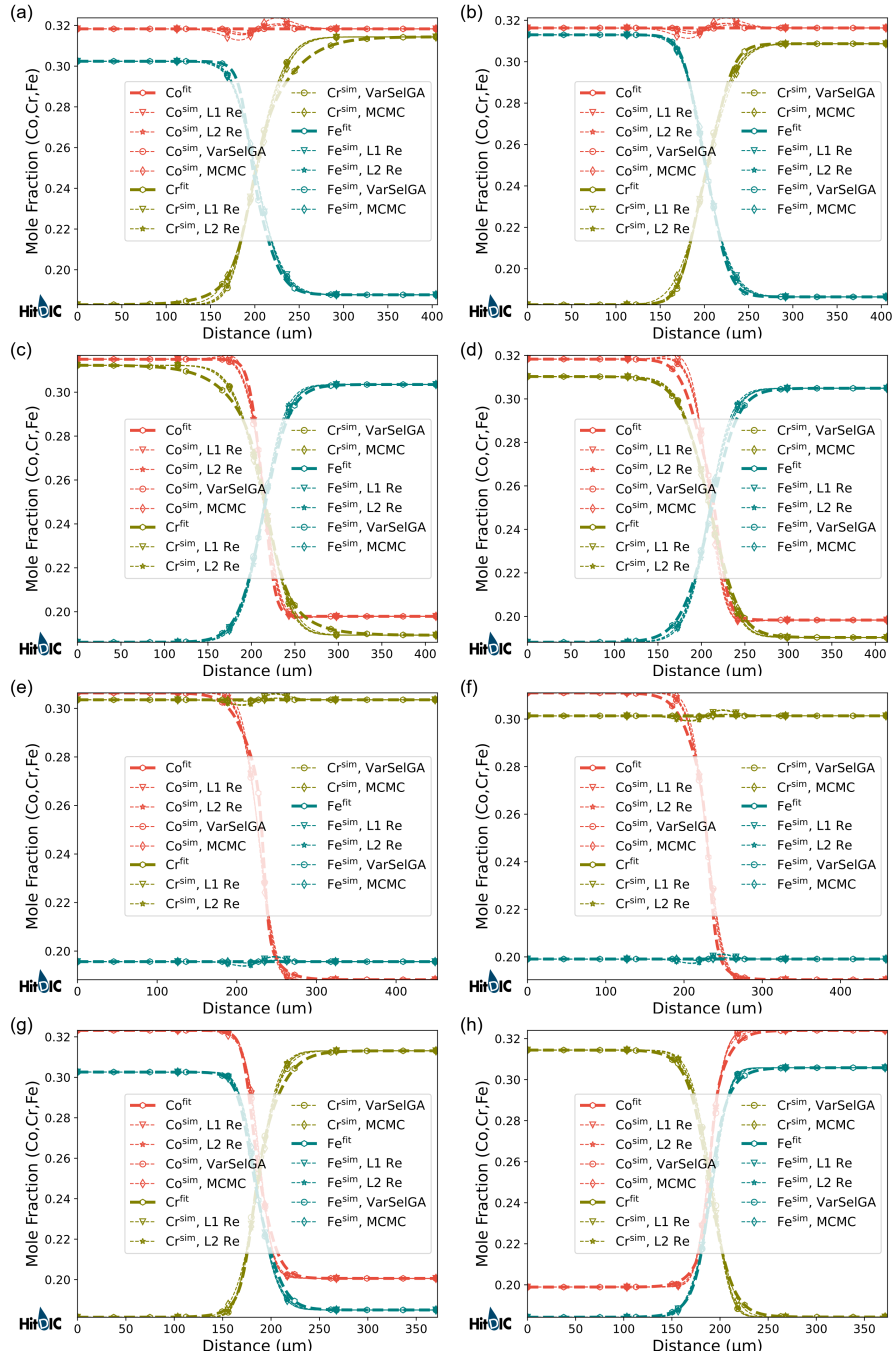
[a27] R. Wang, On the determination of diffusion coefficients and sluggish diffusion effect of face-centered cubic Co-Cr-Fe-Ni-X (X=Mn,Cu) high entropy alloys, Master thesis (2018).



Supplementary Figure 32: Comprison between fitted observations and predictions based on results optimized using different algorithms, i.e., variable selection genetic algorithm (VarSelGA), L1 norm regularization (L1 Re), L2 norm regularization (L2 Re), and Markov chain Monte Carlo (MCMC): The composition profiles of the fitted data (noted as fit) are ported from: (a)-(d) [b1], (e)-(h) [b2]

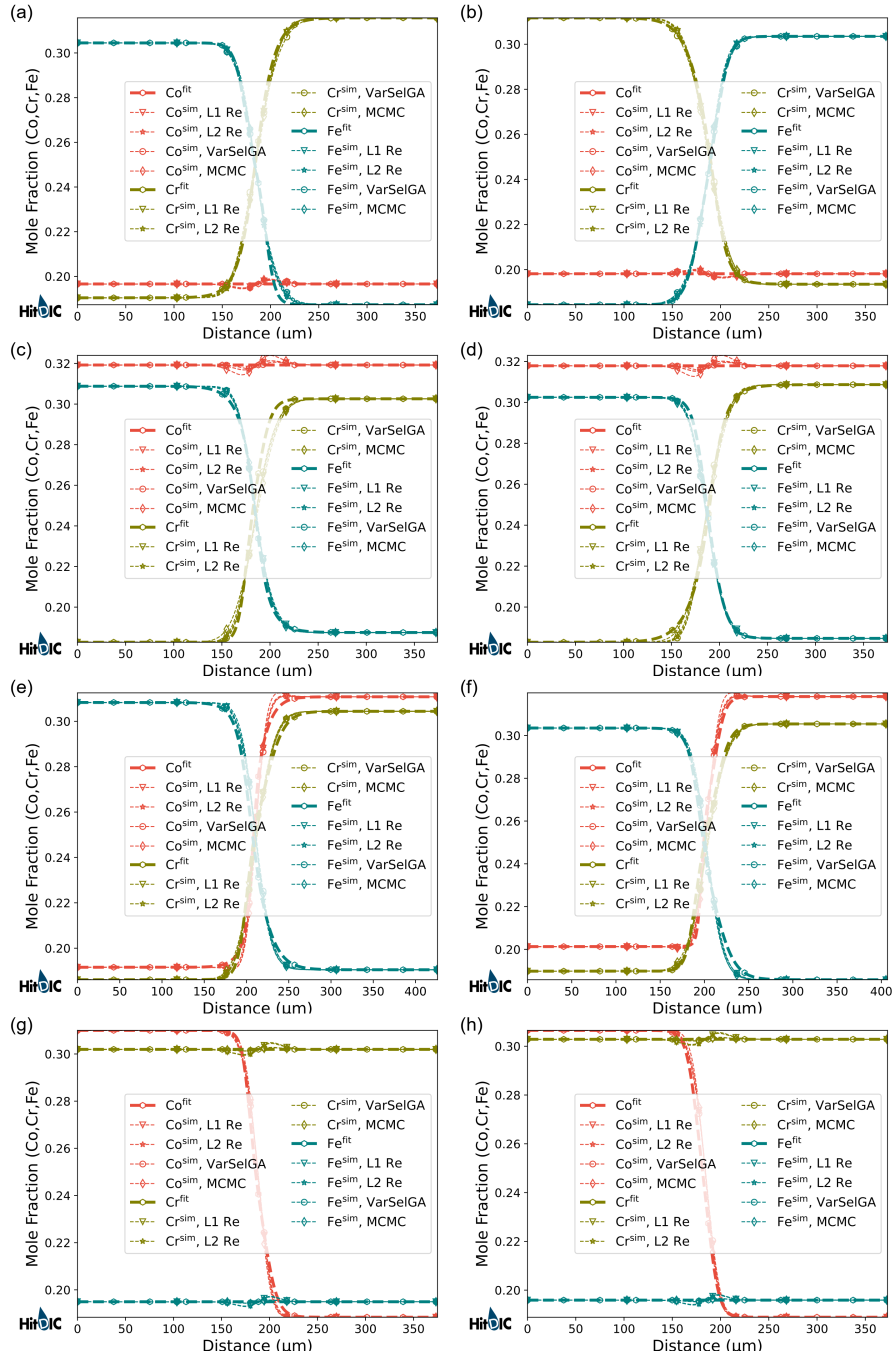
[b1] Chen, W. & Zhang, L. High-Throughput Determination of Interdiffusion Coefficients for Co-Cr-Fe-Mn-Ni High-Entropy Alloys. *J. Phase Equilib. Diffus.* 38, 457–465 (2017).

[b2] Dąbrowa, J. et al. Demystifying the sluggish diffusion effect in high entropy alloys. *J. Alloys Compd.* 783, 193–207 (2019).



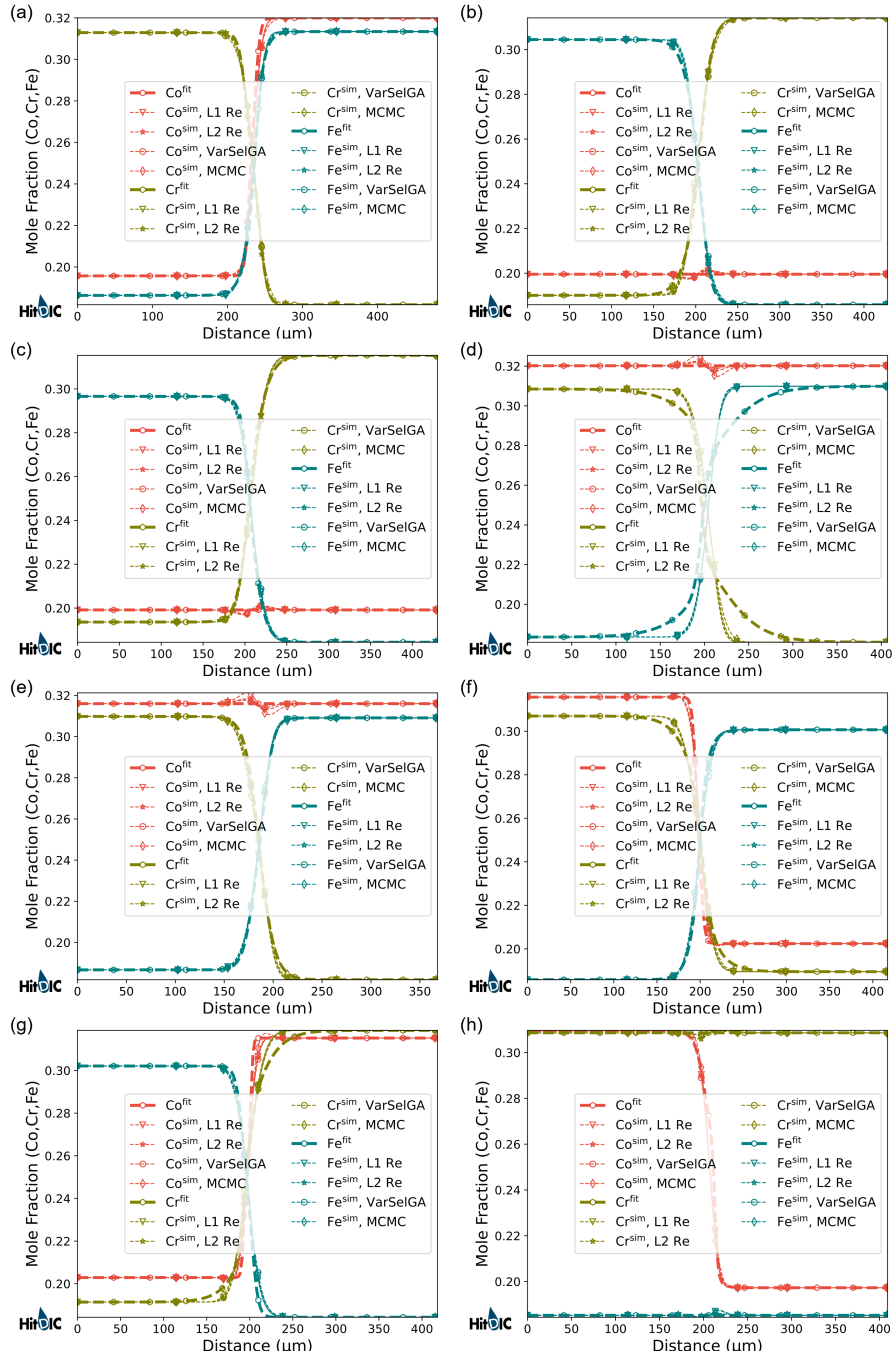
Supplementary Figure 33: Comprison between fitted observations and predictions based on results optimized using different algorithms, i.e., variable selection genetic algorithm (VarSelGA), L1 norm regularization (L1 Re), L2 norm regularization (L2 Re), and Markov chain Monte Carlo (MCMC): The composition profiles of the fitted data (noted as fit) are ported from: (a)-(h) [b3]

[b3] Dąbrowa, J. et al. Demystifying the sluggish diffusion effect in high entropy alloys. J. Alloys Compd. 783, 193–207 (2019).



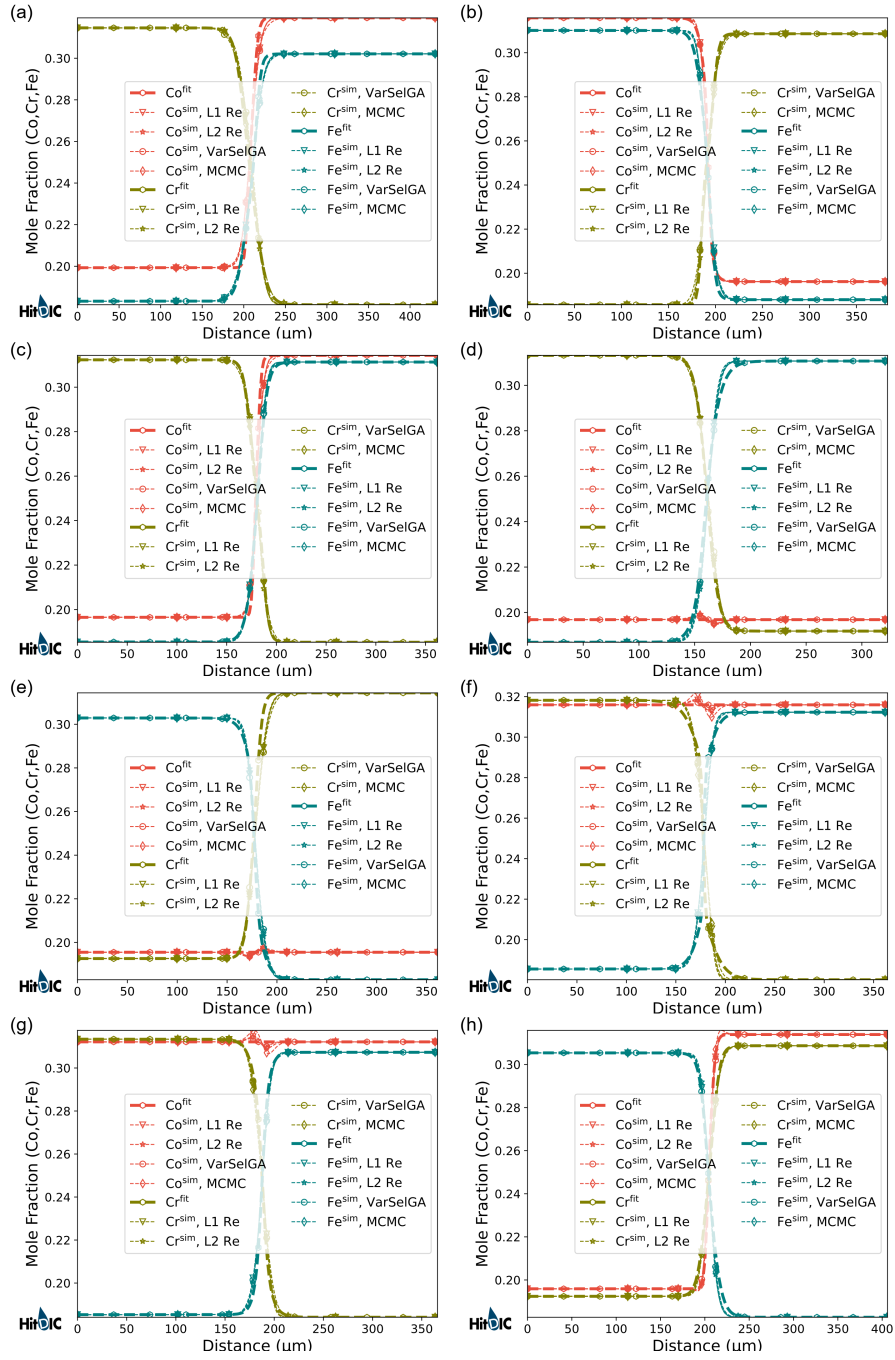
Supplementary Figure 34: Comprison between fitted observations and predictions based on results optimized using different algorithms, i.e., variable selection genetic algorithm (VarSelGA), L1 norm regularization (L1 Re), L2 norm regularization (L2 Re), and Markov chain Monte Carlo (MCMC): The composition profiles of the fitted data (noted as fit) are ported from: (a)-(h) [b4]

[b4] Dąbrowa, J. et al. Demystifying the sluggish diffusion effect in high entropy alloys. J. Alloys Compd. 783, 193–207 (2019).



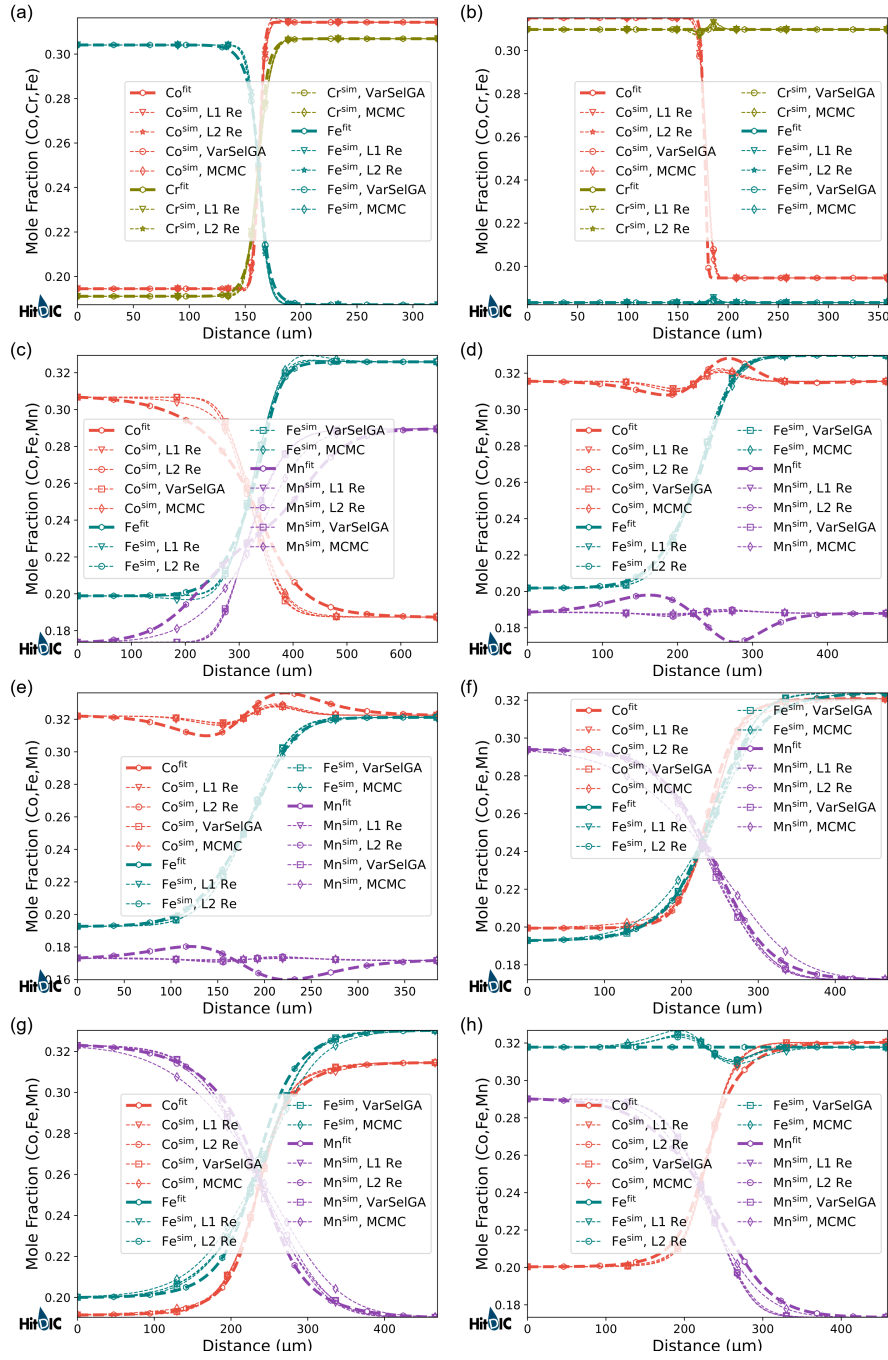
Supplementary Figure 35: Comprison between fitted observations and predictions based on results optimized using different algorithms, i.e., variable selection genetic algorithm (VarSelGA), L1 norm regularization (L1 Re), L2 norm regularization (L2 Re), and Markov chain Monte Carlo (MCMC): The composition profiles of the fitted data (noted as fit) are ported from: (a)-(h) [b5]

[b5] Dąbrowa, J. et al. Demystifying the sluggish diffusion effect in high entropy alloys. *J. Alloys Compd.* 783, 193–207 (2019).



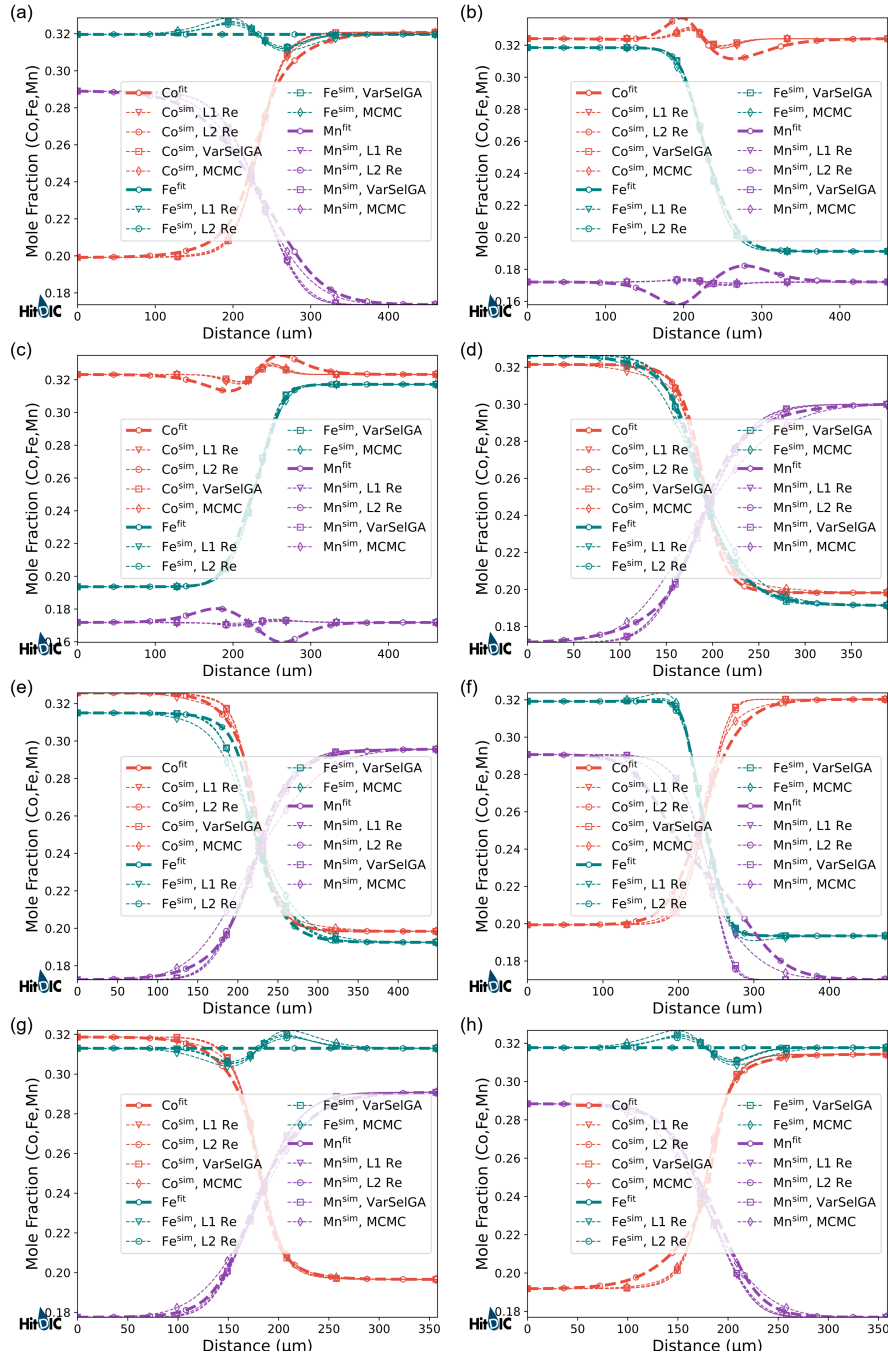
Supplementary Figure 36: Comprison between fitted observations and predictions based on results optimized using different algorithms, i.e., variable selection genetic algorithm (VarSelGA), L1 norm regularization (L1 Re), L2 norm regularization (L2 Re), and Markov chain Monte Carlo (MCMC): The composition profiles of the fitted data (noted as fit) are ported from: (a)-(h) [b6]

[b6] Dąbrowa, J. et al. Demystifying the sluggish diffusion effect in high entropy alloys. *J. Alloys Compd.* 783, 193–207 (2019).



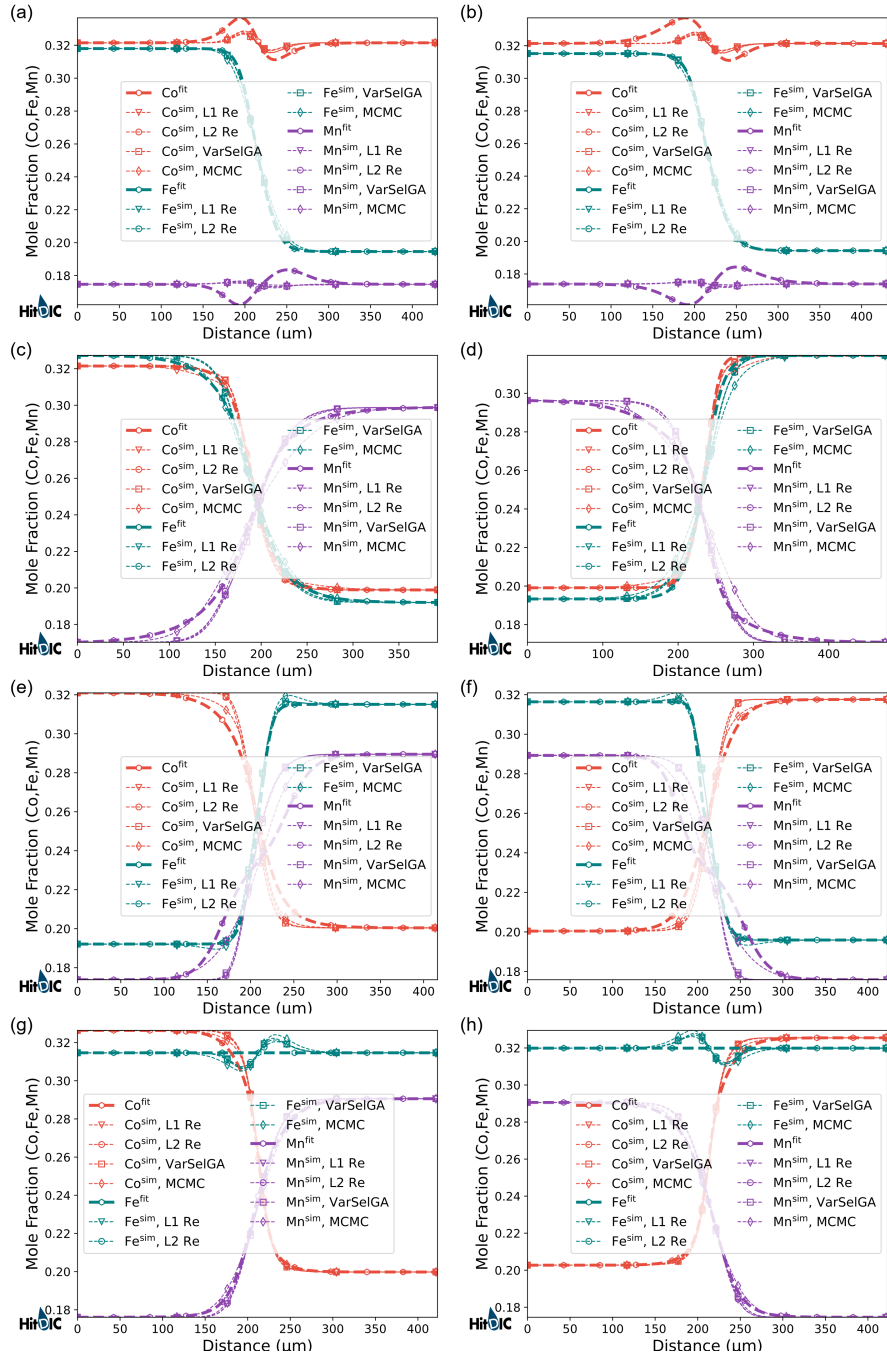
Supplementary Figure 37: Comprison between fitted observations and predictions based on results optimized using different algorithms, i.e., variable selection genetic algorithm (VarSelGA), L1 norm regularization (L1 Re), L2 norm regularization (L2 Re), and Markov chain Monte Carlo (MCMC): The composition profiles of the fitted data (noted as fit) are ported from: (a)-(h) [b7]

[b7] Dąbrowa, J. et al. Demystifying the sluggish diffusion effect in high entropy alloys. *J. Alloys Compd.* 783, 193–207 (2019).



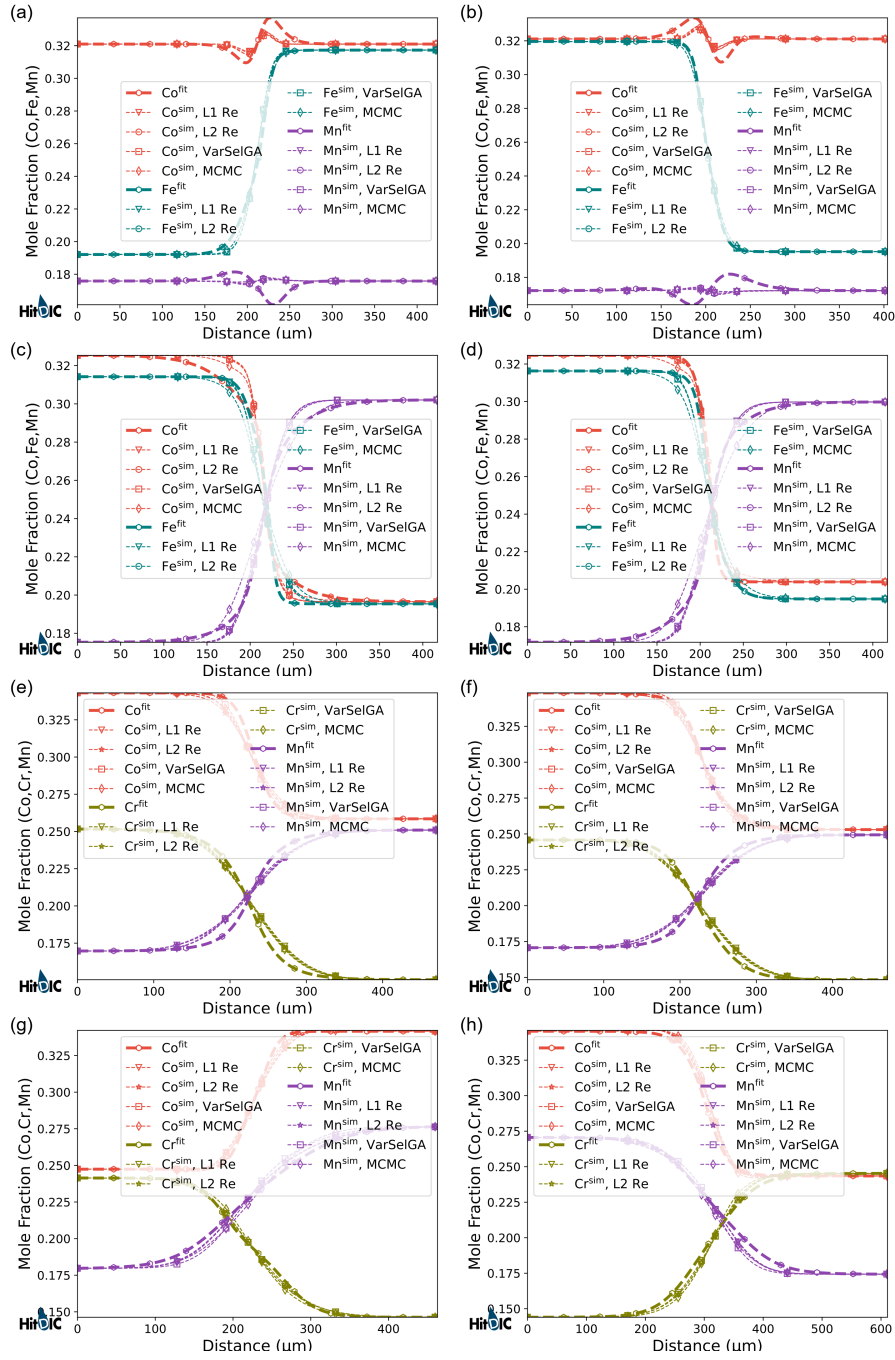
Supplementary Figure 38: Comprison between fitted observations and predictions based on results optimized using different algorithms, i.e., variable selection genetic algorithm (VarSelGA), L1 norm regularization (L1 Re), L2 norm regularization (L2 Re), and Markov chain Monte Carlo (MCMC): The composition profiles of the fitted data (noted as fit) are ported from: (a)-(h) [b8]

[b8] Dąbrowa, J. et al. Demystifying the sluggish diffusion effect in high entropy alloys. J. Alloys Compd. 783, 193–207 (2019).



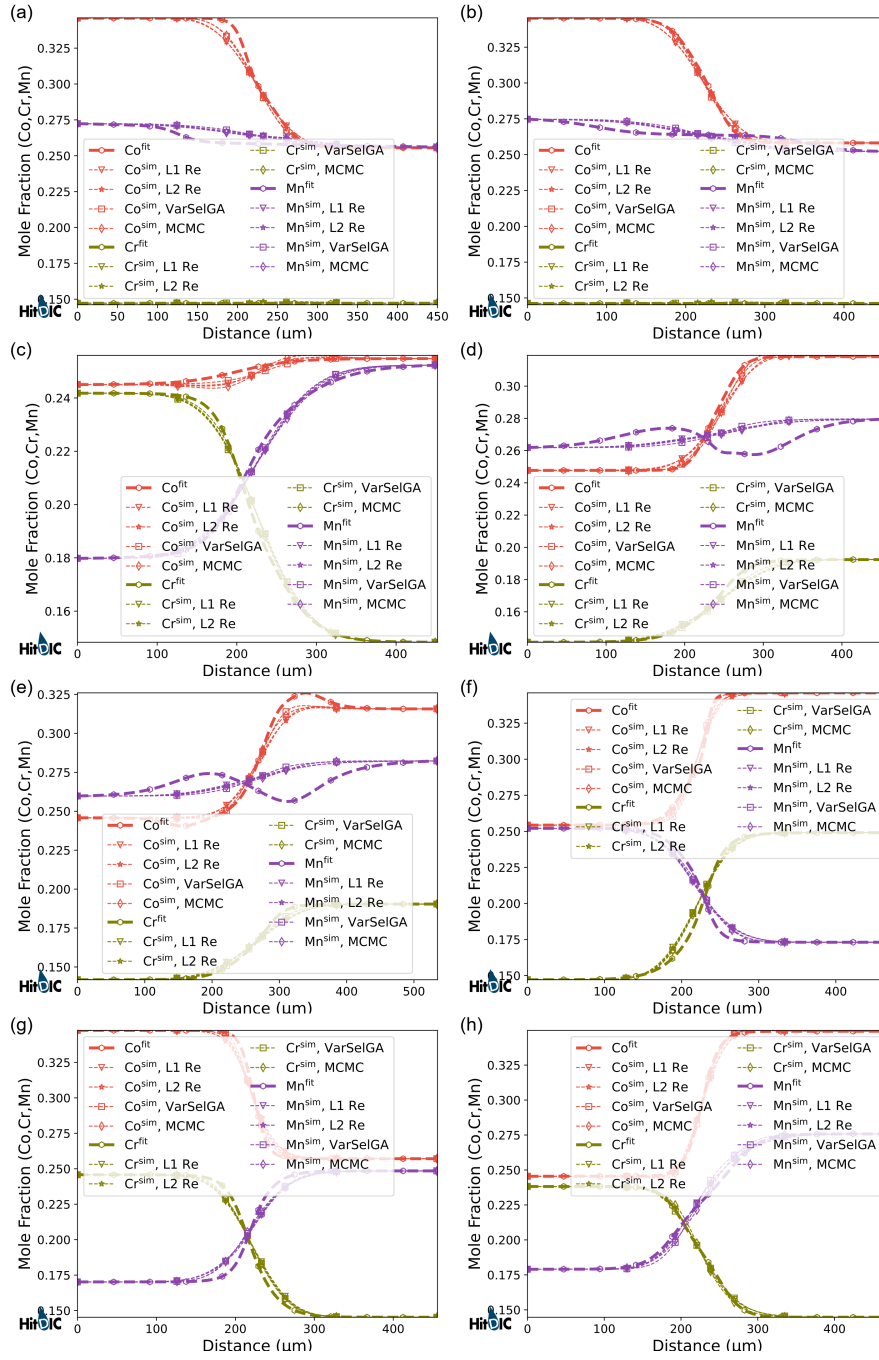
Supplementary Figure 39: Comprison between fitted observations and predictions based on results optimized using different algorithms, i.e., variable selection genetic algorithm (VarSelGA), L1 norm regularization (L1 Re), L2 norm regularization (L2 Re), and Markov chain Monte Carlo (MCMC): The composition profiles of the fitted data (noted as fit) are ported from: (a)-(h) [b9]

[b9] Dąbrowa, J. et al. Demystifying the sluggish diffusion effect in high entropy alloys. J. Alloys Compd. 783, 193–207 (2019).



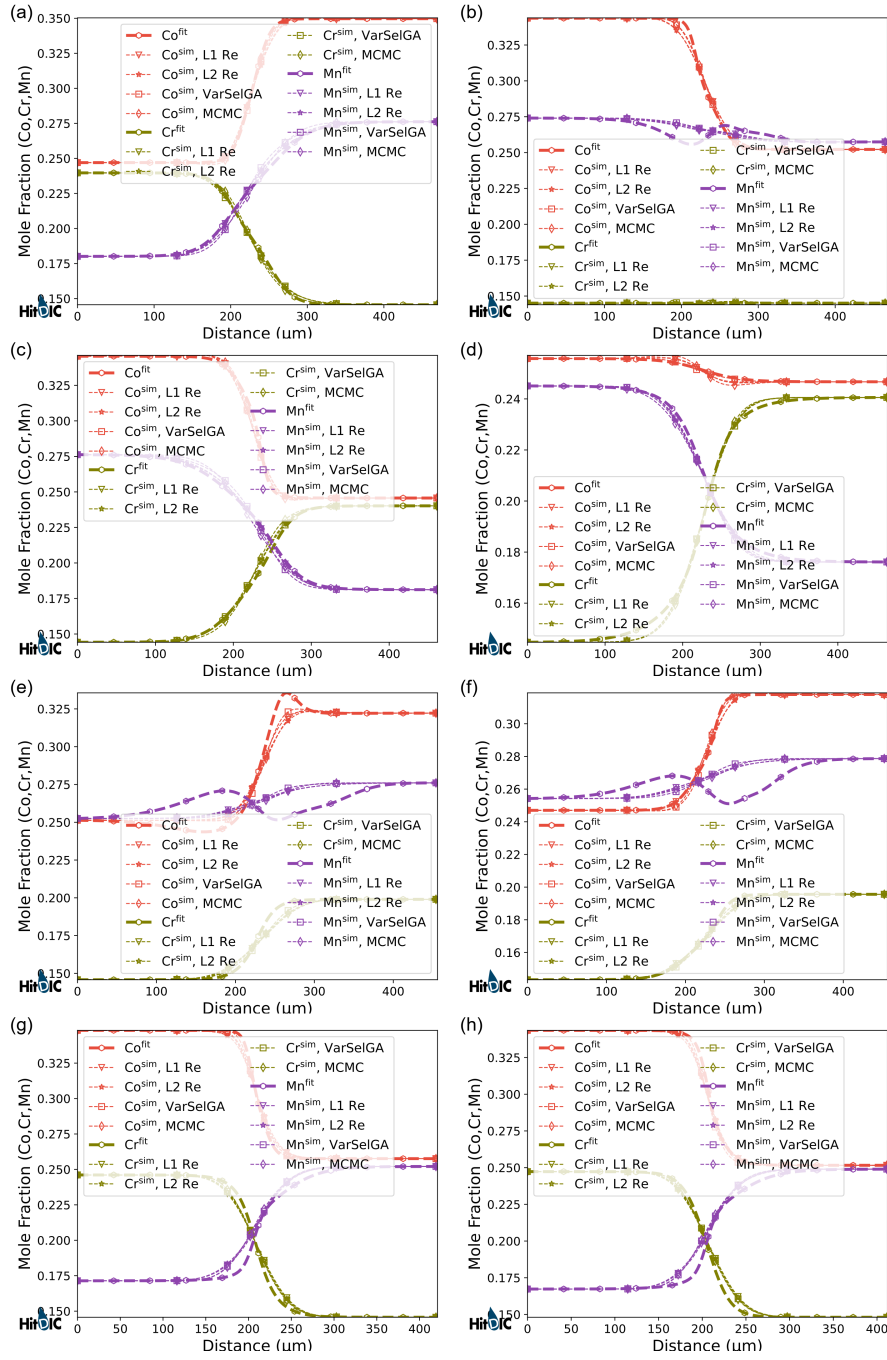
Supplementary Figure 40: Comprison between fitted observations and predictions based on results optimized using different algorithms, i.e., variable selection genetic algorithm (VarSelGA), L1 norm regularization (L1 Re), L2 norm regularization (L2 Re), and Markov chain Monte Carlo (MCMC): The composition profiles of the fitted data (noted as fit) are ported from: (a)-(h) [b10]

[b10] Dąbrowa, J. et al. Demystifying the sluggish diffusion effect in high entropy alloys. *J. Alloys Compd.* 783, 193–207 (2019).



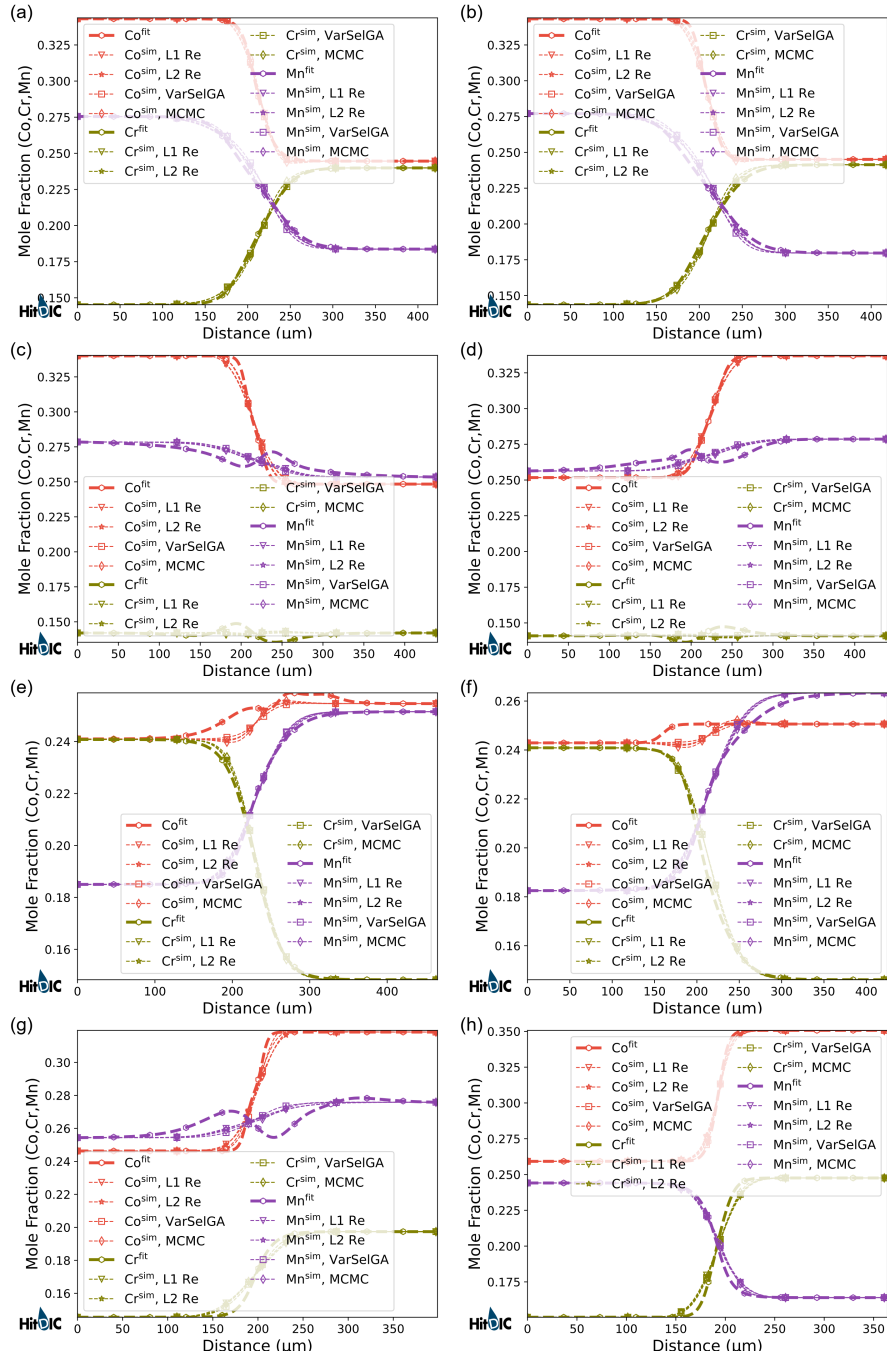
Supplementary Figure 41: Comprison between fitted observations and predictions based on results optimized using different algorithms, i.e., variable selection genetic algorithm (VarSelGA), L1 norm regularization (L1 Re), L2 norm regularization (L2 Re), and Markov chain Monte Carlo (MCMC): The composition profiles of the fitted data (noted as fit) are ported from: (a)-(h) [b11]

[b11] Dąbrowa, J. et al. Demystifying the sluggish diffusion effect in high entropy alloys. *J. Alloys Compd.* 783, 193–207 (2019).



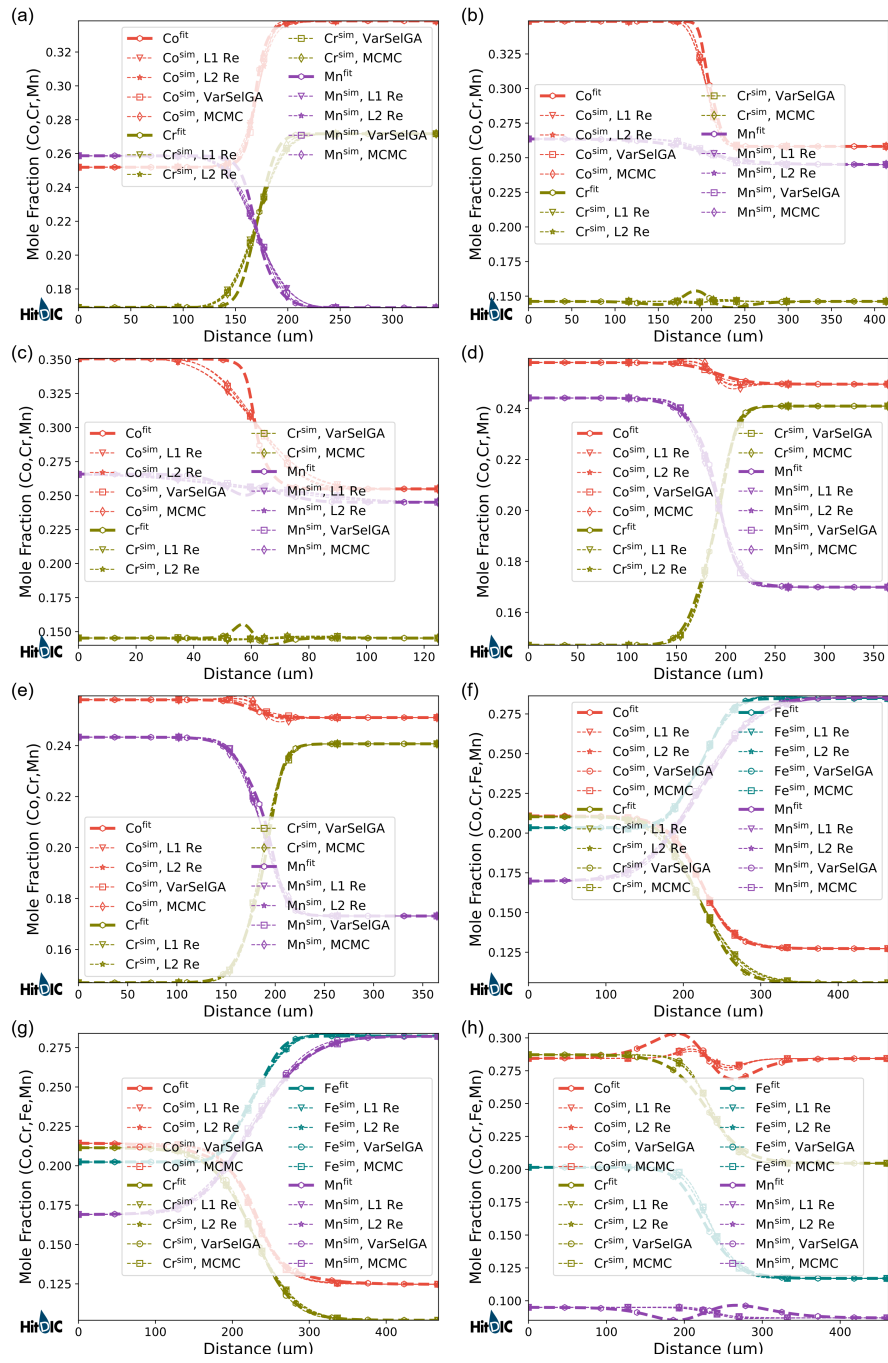
Supplementary Figure 42: Comprison between fitted observations and predictions based on results optimized using different algorithms, i.e., variable selection genetic algorithm (VarSelGA), L1 norm regularization (L1 Re), L2 norm regularization (L2 Re), and Markov chain Monte Carlo (MCMC): The composition profiles of the fitted data (noted as fit) are ported from: (a)-(h) [b12]

[b12] Dąbrowa, J. et al. Demystifying the sluggish diffusion effect in high entropy alloys. *J. Alloys Compd.* 783, 193–207 (2019).



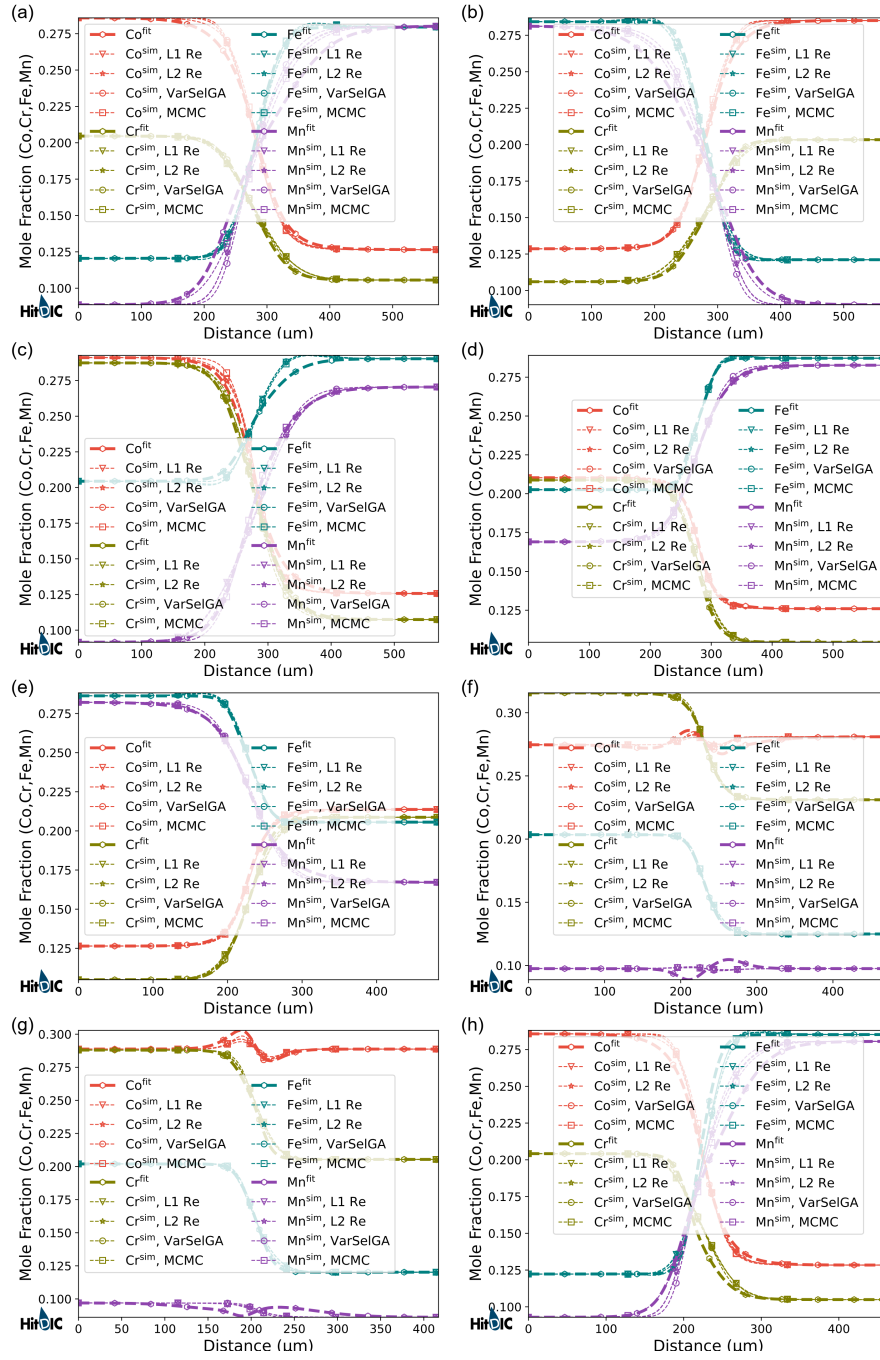
Supplementary Figure 43: Comprison between fitted observations and predictions based on results optimized using different algorithms, i.e., variable selection genetic algorithm (VarSelGA), L1 norm regularization (L1 Re), L2 norm regularization (L2 Re), and Markov chain Monte Carlo (MCMC): The composition profiles of the fitted data (noted as fit) are ported from: (a)-(h) [b13]

[b13] Dąbrowa, J. et al. Demystifying the sluggish diffusion effect in high entropy alloys. *J. Alloys Compd.* 783, 193–207 (2019).



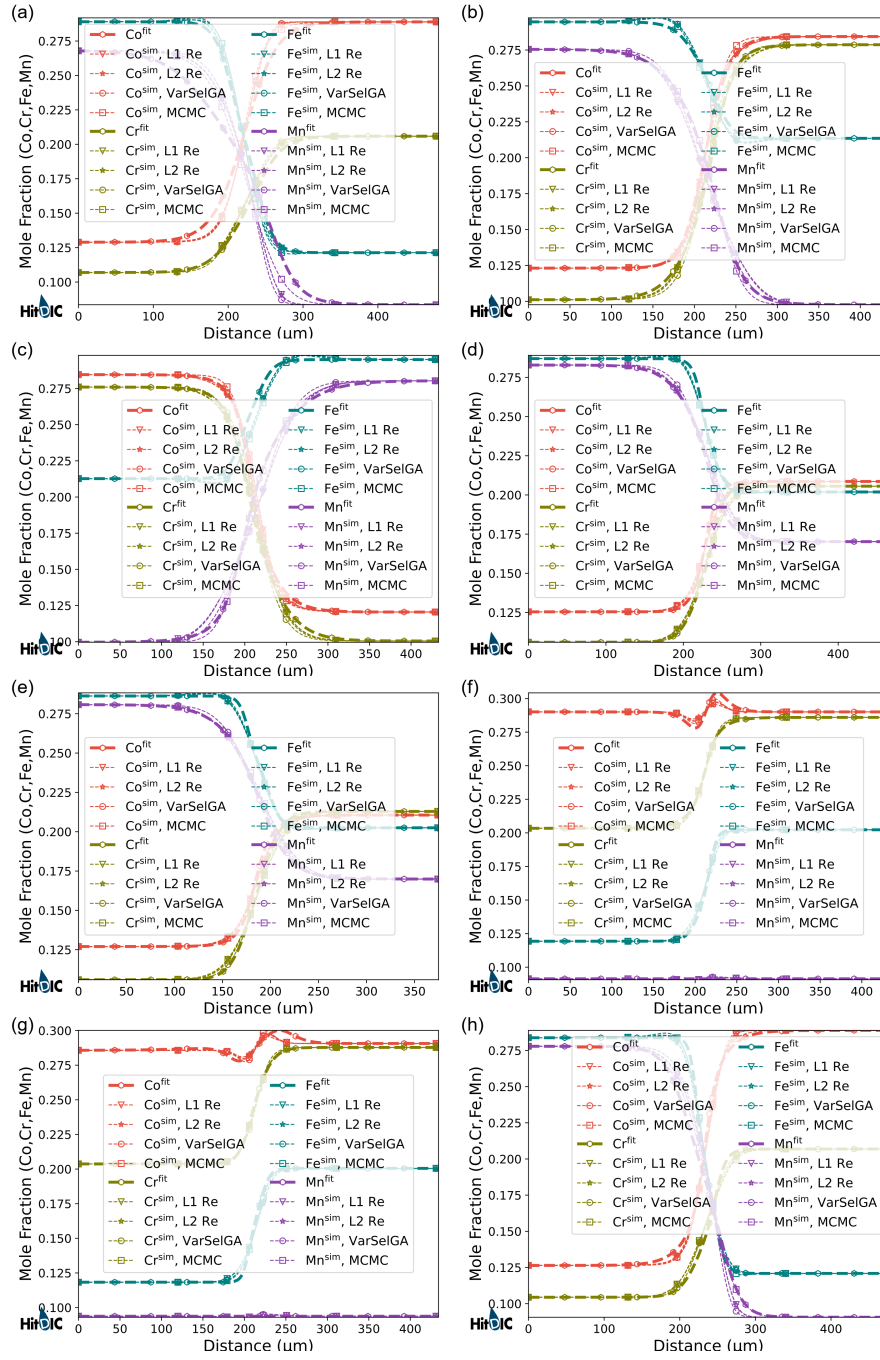
Supplementary Figure 44: Comprison between fitted observations and predictions based on results optimized using different algorithms, i.e., variable selection genetic algorithm (VarSelGA), L1 norm regularization (L1 Re), L2 norm regularization (L2 Re), and Markov chain Monte Carlo (MCMC): The composition profiles of the fitted data (noted as fit) are ported from: (a)-(h) [b14]

[b14] Dąbrowa, J. et al. Demystifying the sluggish diffusion effect in high entropy alloys. *J. Alloys Compd.* 783, 193–207 (2019).



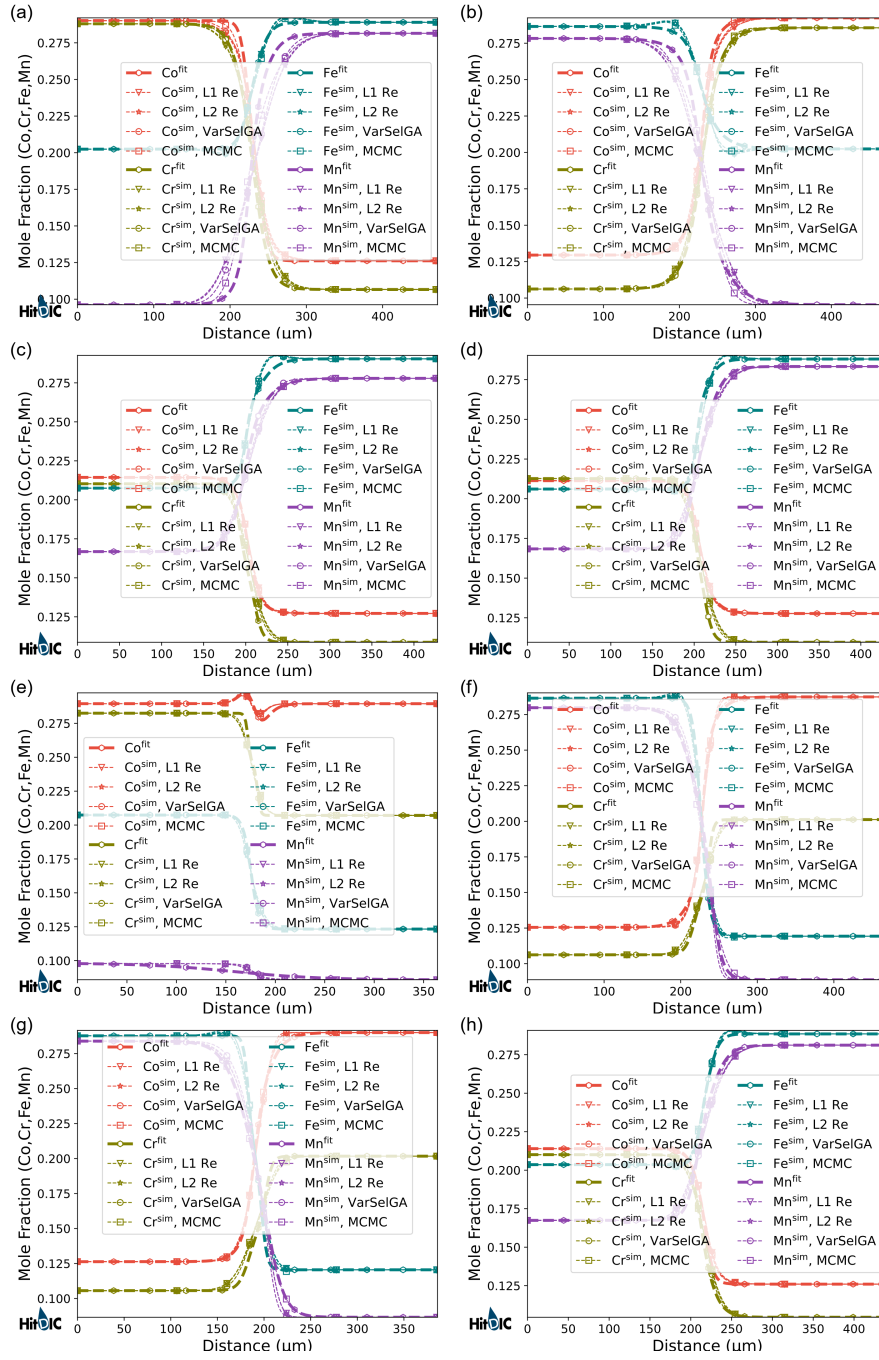
Supplementary Figure 45: Comprison between fitted observations and predictions based on results optimized using different algorithms, i.e., variable selection genetic algorithm (VarSelGA), L1 norm regularization (L1 Re), L2 norm regularization (L2 Re), and Markov chain Monte Carlo (MCMC): The composition profiles of the fitted data (noted as fit) are ported from: (a)-(h) [b15]

[b15] Dąbrowa, J. et al. Demystifying the sluggish diffusion effect in high entropy alloys. *J. Alloys Compd.* 783, 193–207 (2019).



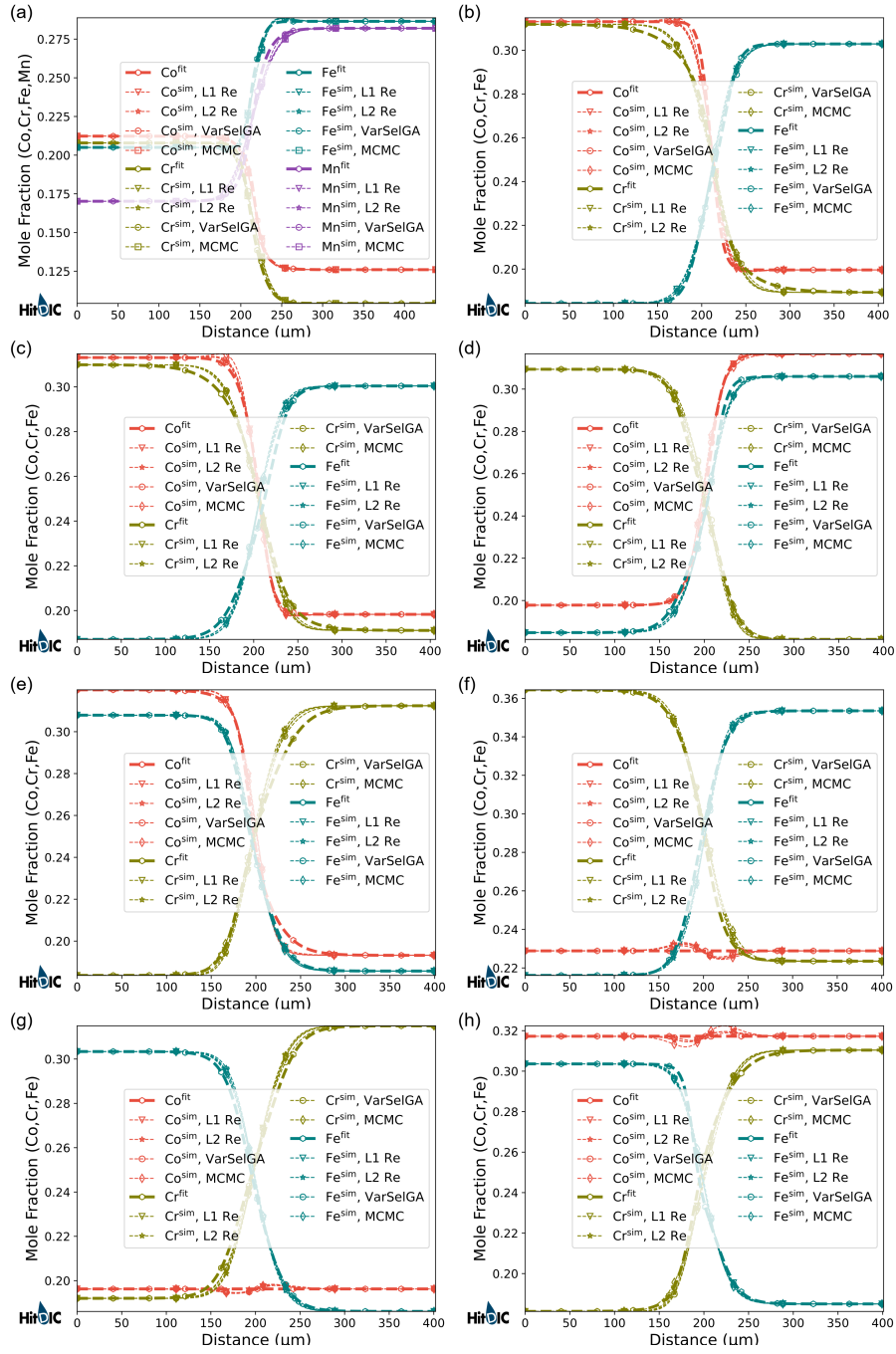
Supplementary Figure 46: Comprison between fitted observations and predictions based on results optimized using different algorithms, i.e., variable selection genetic algorithm (VarSelGA), L1 norm regularization (L1 Re), L2 norm regularization (L2 Re), and Markov chain Monte Carlo (MCMC): The composition profiles of the fitted data (noted as fit) are ported from: (a)-(h) [b16]

[b16] Dąbrowa, J. et al. Demystifying the sluggish diffusion effect in high entropy alloys. *J. Alloys Compd.* 783, 193–207 (2019).



Supplementary Figure 47: Comprison between fitted observations and predictions based on results optimized using different algorithms, i.e., variable selection genetic algorithm (VarSelGA), L1 norm regularization (L1 Re), L2 norm regularization (L2 Re), and Markov chain Monte Carlo (MCMC): The composition profiles of the fitted data (noted as fit) are ported from: (a)-(h) [b17]

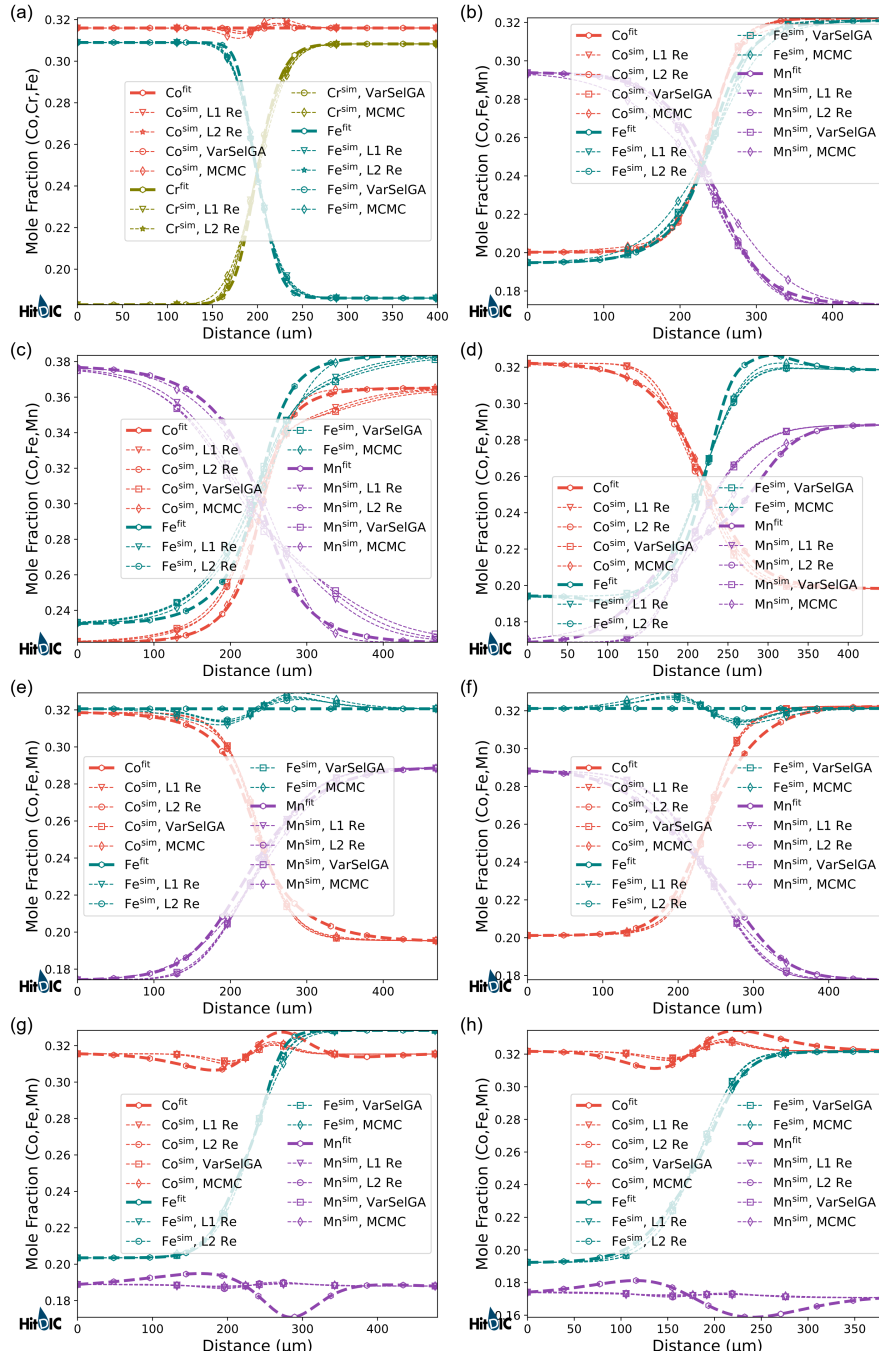
[b17] Dąbrowa, J. et al. Demystifying the sluggish diffusion effect in high entropy alloys. *J. Alloys Compd.* 783, 193–207 (2019).



Supplementary Figure 48: Comprison between fitted observations and predictions based on results optimized using different algorithms, i.e., variable selection genetic algorithm (VarSelGA), L1 norm regularization (L1 Re), L2 norm regularization (L2 Re), and Markov chain Monte Carlo (MCMC): The composition profiles of the fitted data (noted as fit) are ported from: (a) [b18], (b)-(h) [b19]

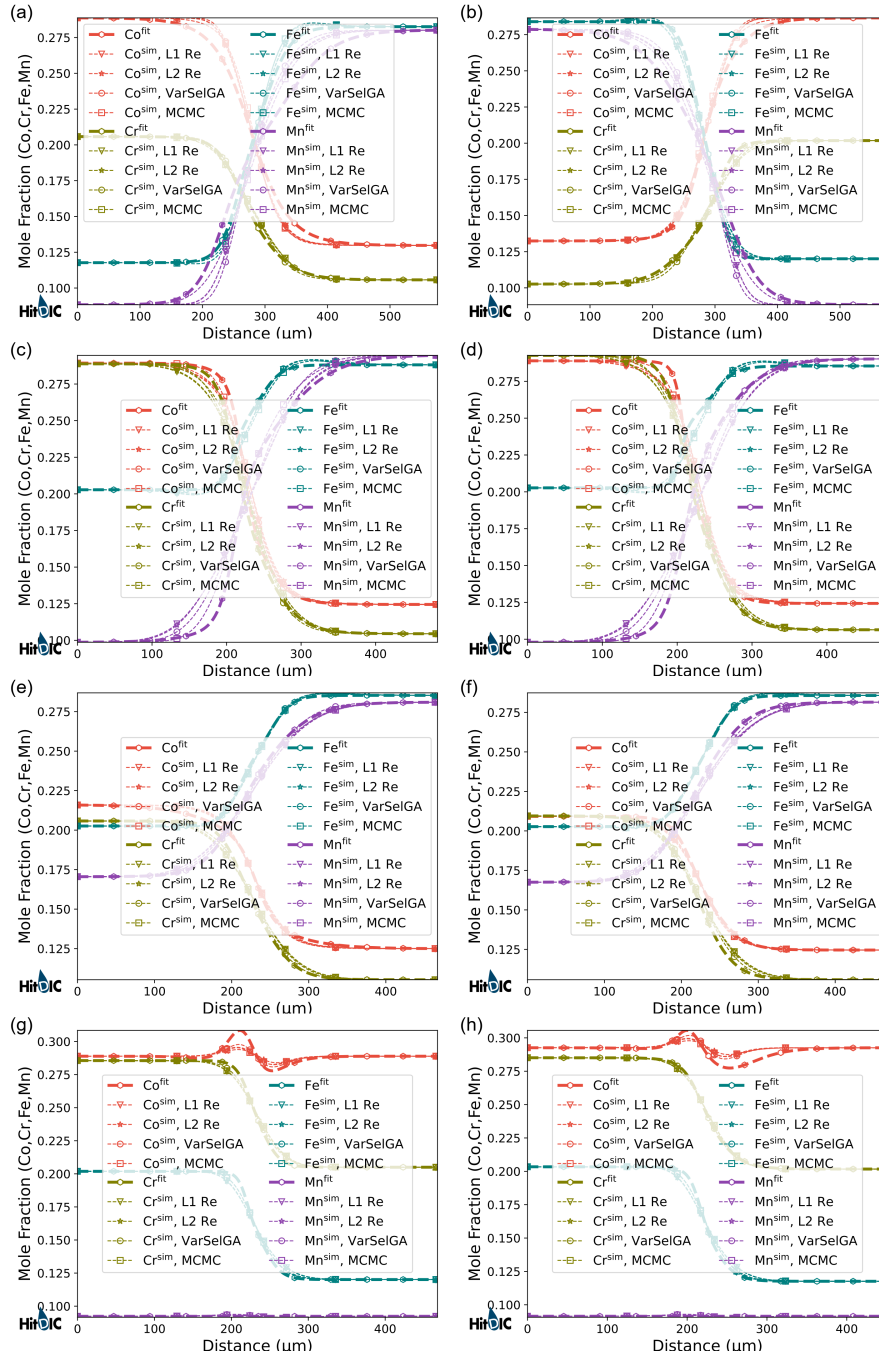
[b18] Dąbrowa, J. et al. Demystifying the sluggish diffusion effect in high entropy alloys. *J. Alloys Compd.* 783, 193–207 (2019).

[b19] Kucza, W. et al. Studies of “sluggish diffusion” effect in Co-Cr-Fe-Mn-Ni, Co-Cr-Fe-Ni and Co-Fe-Mn-Ni high entropy alloys; determination of tracer diffusivities by combinatorial approach. *J. Alloys Compd.* 731, 920–928 (2018).



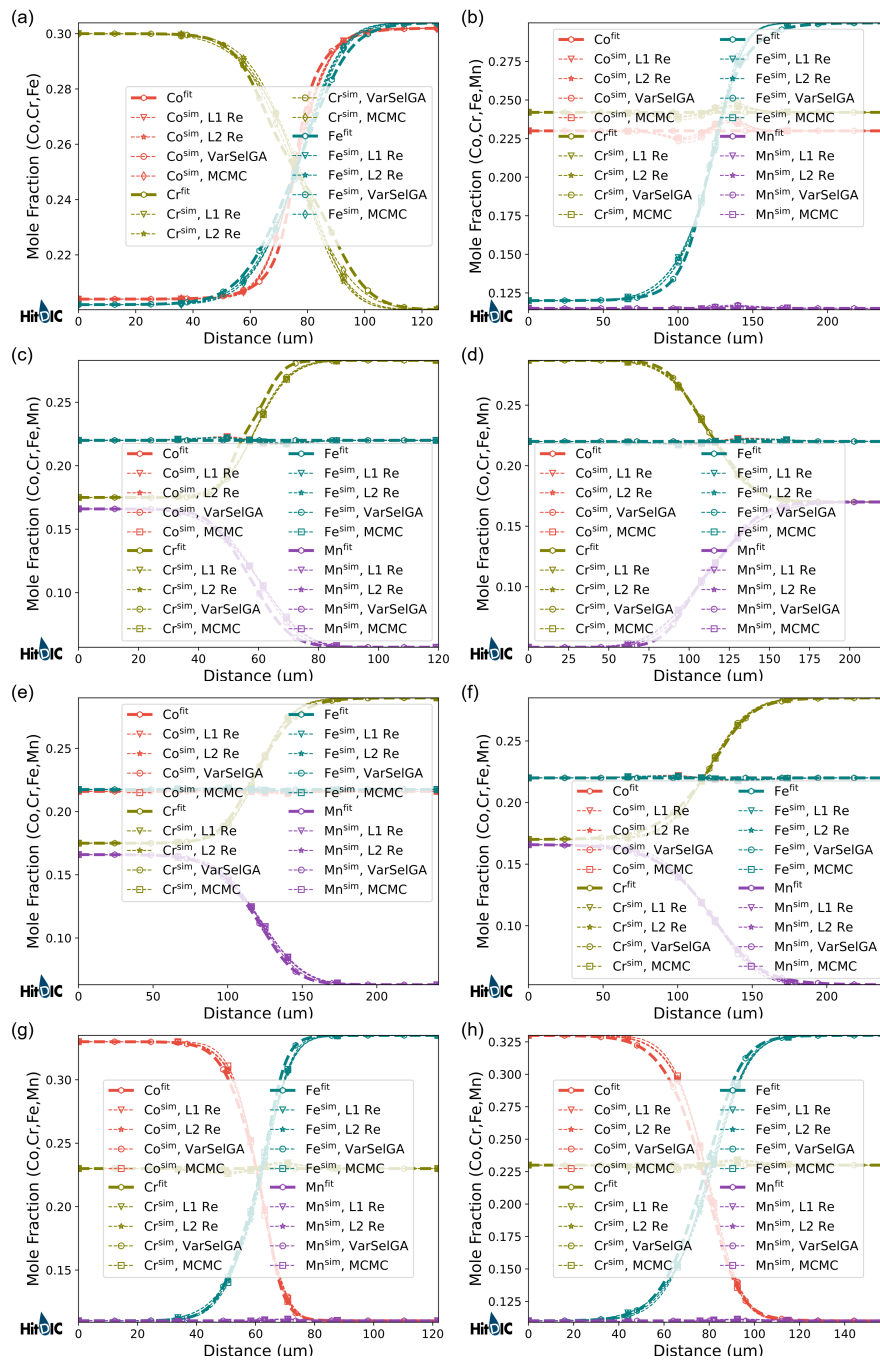
Supplementary Figure 49: Comprison between fitted observations and predictions based on results optimized using different algorithms, i.e., variable selection genetic algorithm (VarSelGA), L1 norm regularization (L1 Re), L2 norm regularization (L2 Re), and Markov chain Monte Carlo (MCMC): The composition profiles of the fitted data (noted as fit) are ported from: (a)-(h) [b20]

[b20] Kucza, W. et al. Studies of “sluggish diffusion” effect in Co-Cr-Fe-Mn-Ni, Co-Cr-Fe-Ni and Co-Fe-Mn-Ni high entropy alloys; determination of tracer diffusivities by combinatorial approach. J. Alloys Compd. 731, 920–928 (2018).



Supplementary Figure 50: Comprison between fitted observations and predictions based on results optimized using different algorithms, i.e., variable selection genetic algorithm (VarSelGA), L1 norm regularization (L1 Re), L2 norm regularization (L2 Re), and Markov chain Monte Carlo (MCMC): The composition profiles of the fitted data (noted as fit) are ported from: (a)-(h) [b21]

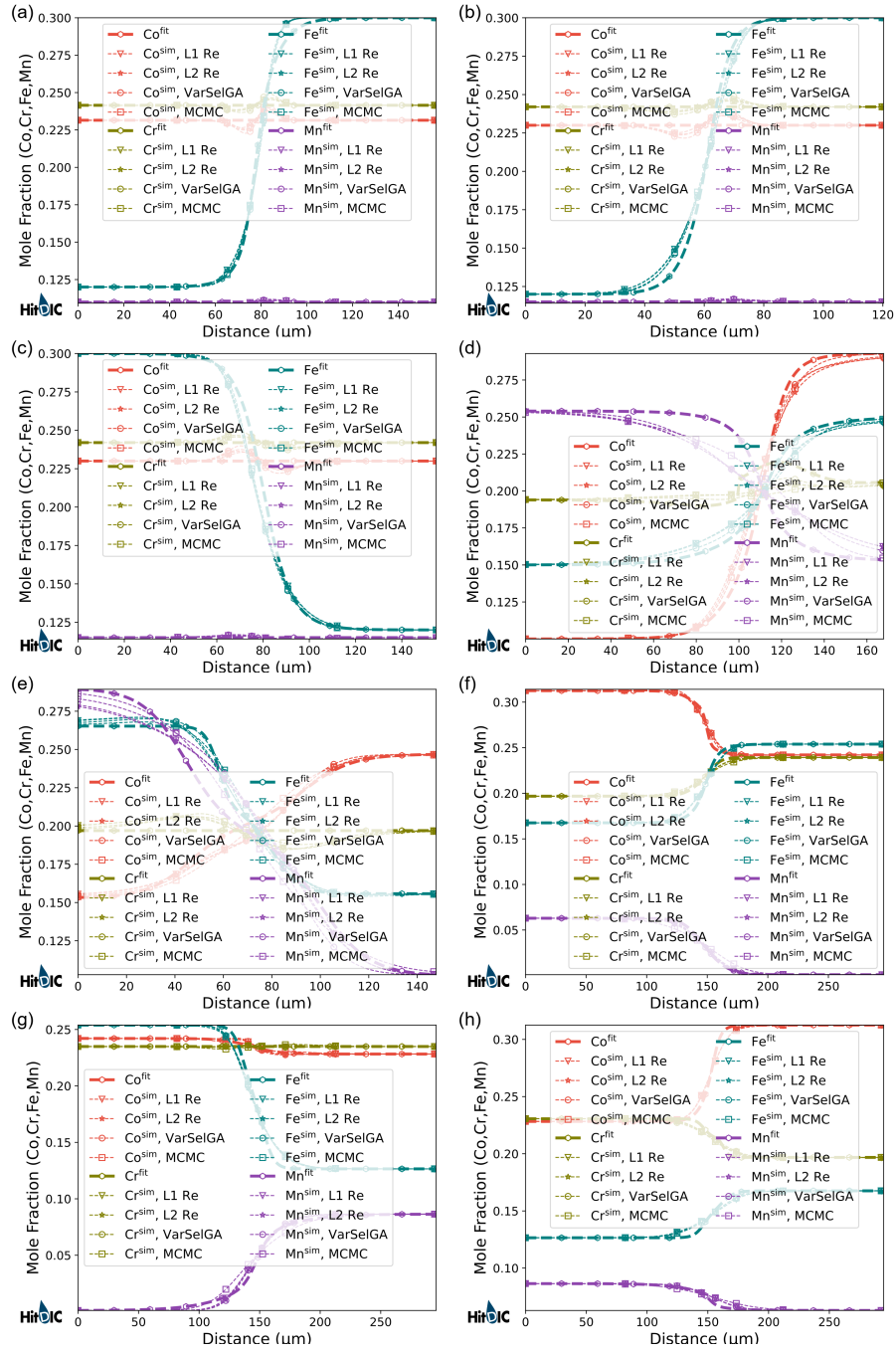
[b21] Kucza, W. et al. Studies of “sluggish diffusion” effect in Co-Cr-Fe-Mn-Ni, Co-Cr-Fe-Ni and Co-Fe-Mn-Ni high entropy alloys; determination of tracer diffusivities by combinatorial approach. J. Alloys Compd. 731, 920–928 (2018).



Supplementary Figure 51: Comprison between fitted observations and predictions based on results optimized using different algorithms, i.e., variable selection genetic algorithm (VarSelGA), L1 norm regularization (L1 Re), L2 norm regularization (L2 Re), and Markov chain Monte Carlo (MCMC): The composition profiles of the fitted data (noted as fit) are ported from: (a) [b22], (b)-(h) [b23]

[b22] Kulkarni, K. & Chauhan, G. P. S. Investigations of quaternary interdiffusion in a constituent system of high entropy alloys. AIP Advances 5, 097162 (2015).

[b23] Tsai, K.-Y., Tsai, M.-H. & Yeh, J.-W. Sluggish diffusion in Co–Cr–Fe–Mn–Ni high-entropy alloys. Acta Mater. 61, 4887–4897 (2013).

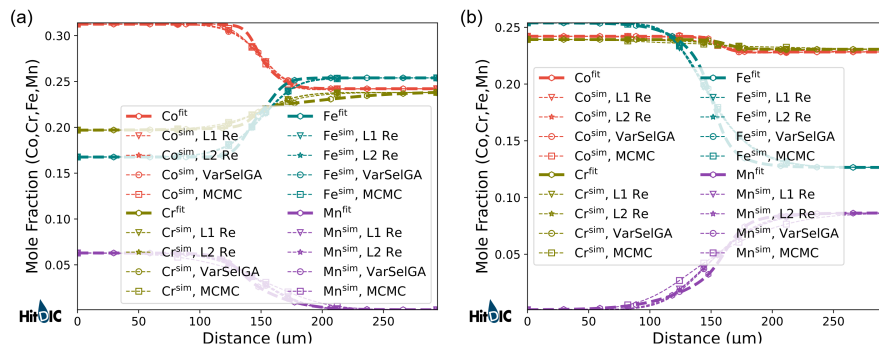


Supplementary Figure 52: Comprison between fitted observations and predictions based on results optimized using different algorithms, i.e., variable selection genetic algorithm (VarSelGA), L1 norm regularization (L1 Re), L2 norm regularization (L2 Re), and Markov chain Monte Carlo (MCMC): The composition profiles of the fitted data (noted as fit) are ported from: (a)-(c) [b24], (d)-(e) [b25], (f)-(h) [b26]

[b24] Tsai, K.-Y., Tsai, M.-H. & Yeh, J.-W. Sluggish diffusion in Co–Cr–Fe–Mn–Ni high-entropy alloys. *Acta Mater.* 61, 4887–4897 (2013).

[b25] Verma, V., Tripathi, A. & Kulkarni, K. N. On Interdiffusion in FeNiCoCrMn High Entropy Alloy. *J. Phase Equilib. Diffus.* 38, 445–456 (2017).

[b26] R. Wang, On the determination of diffusion coefficients and sluggish diffusion effect of face-centered cubic Co–Cr–Fe–Ni–X(X=Mn,Cu) high entropy alloys, Master thesis (2018).



Supplementary Figure 53: Comprison between fitted observations and predictions based on results optimized using different algorithms, i.e., variable selection genetic algorithm (VarSelGA), L1 norm regularization (L1 Re), L2 norm regularization (L2 Re), and Markov chain Monte Carlo (MCMC): The composition profiles of the fitted data (noted as fit) are ported from: (a)-(b) [b27]

[b27] R. Wang, On the determination of diffusion coefficients and sluggish diffusion effect of face-centered cubic Co-Cr-Fe-Ni-X(X=Mn,Cu) high entropy alloys, Master thesis (2018).