Supporting Information

Effects of sulfur and mineral elements (Ca, Al, Si and Fe) on thermochemical behaviors of zinc during co-pyrolysis of coal and waste tire: a combined experimental and thermodynamic simulation study

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Table S1. Mass distributions of Zn in the pyrolytic products.

Sample	Sample weight before pyrolysis (g)	Total Zn in sample (g)	Pyrolysis temperature (°C)	Generated coke (g)	Zn in coke (g)	Zn in tar (g)	Zn in gas (g)
WT-2	10.0000	0.2131		3.7334	0.1881	0.0244	6.12×10^{-4}
Coal+3wt.%WT-2	9.9770	0.00759		7.5714	0.0074	1.82×10^{-4}	1.70×10^{-5}
Coal+5wt.%WT-2	9.9851	0.01182	700	7.5145	0.0115	2.19×10^{-4}	9.81×10^{-5}
Coal+1wt.%ZnO	9.9887	0.08139		7.7530	0.0788	0.0024	1.97×10^{-4}
Coal+5wt.%ZnO	9.9828	0.40173		7.7075	0.3627	0.0389	1.31×10^{-4}
WT-2	10.0000	0.2131		3.4744	0.0856	0.1268	6.5×10^{-4}
Coal+3wt.%WT-2	9.9671	0.00758		7.3600	8.96×10^{-4}	0.0066	5.75×10^{-5}
Coal+5wt.%WT-2	9.9834	0.01182	900	7.2507	6.14×10^{-4}	0.0112	4.75×10^{-5}
Coal+1wt.%ZnO	9.9901	0.08140		7.4327	0.0255	0.0556	2.84×10^{-4}
Coal+5wt.%ZnO	9.0050	0.36238		6.5896	0.1845	0.1775	3.34×10^{-4}
WT-2	9.9996	0.2131		3.3162	0.0001	0.2111	0.0019
Coal+3wt.%WT-2	9.9858	0.00759		7.2754	0.0012	0.0064	2.33×10^{-5}
Coal+5wt.%WT-2	9.9916	0.01183	1050	7.2017	0.0016	0.0102	3.70×10^{-5}
Coal+1wt.%ZnO	9.9855	0.08137		7.3796	0.0192	0.0617	3.95×10^{-4}
Coal+5wt.%ZnO	9.9631	0.40094		7.0351	0.0389	0.3610	9.94×10^{-4}

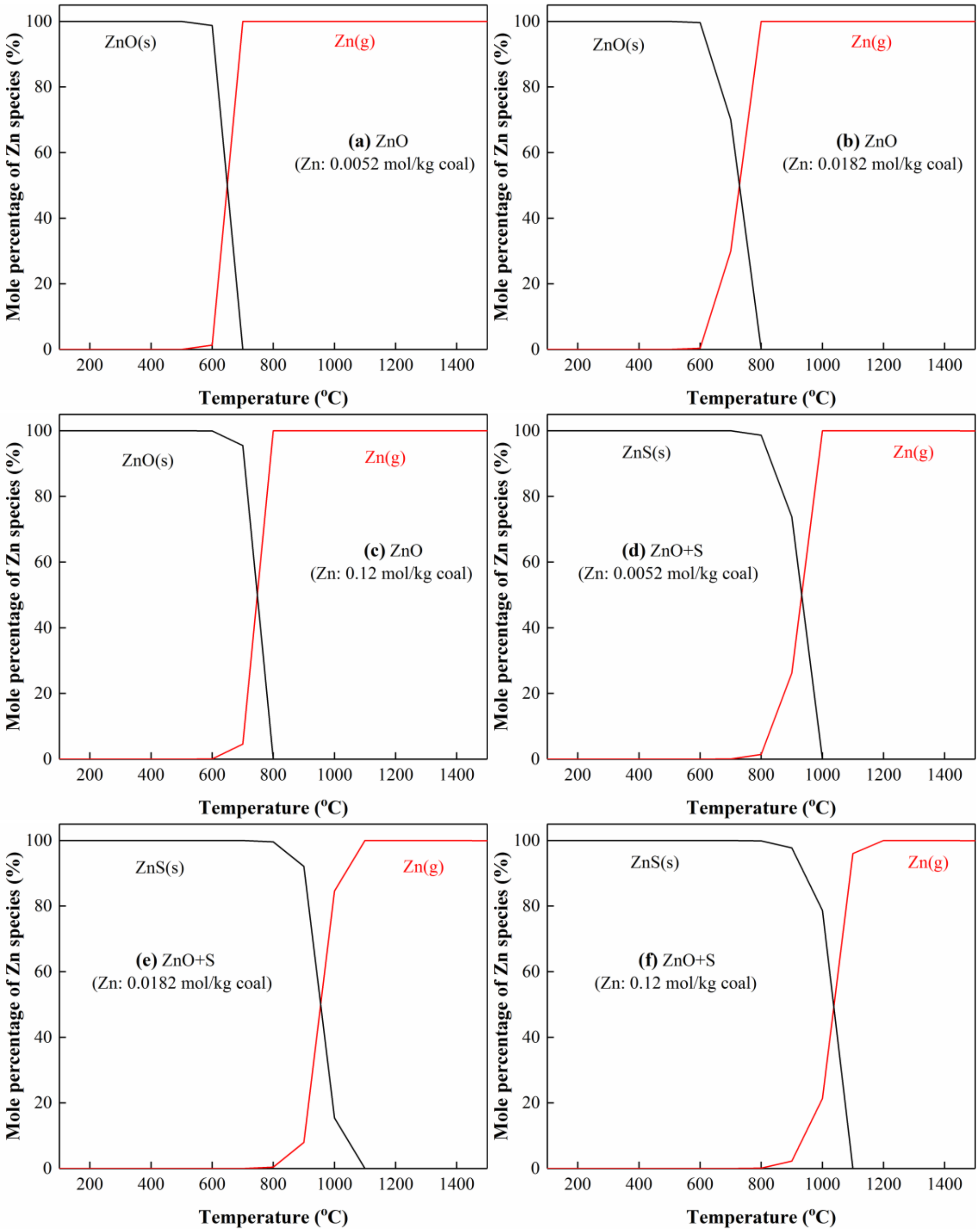

Figure S1. Thermodynamic equilibrium distributions of zinc when sulfur and zinc coexist in the coal.

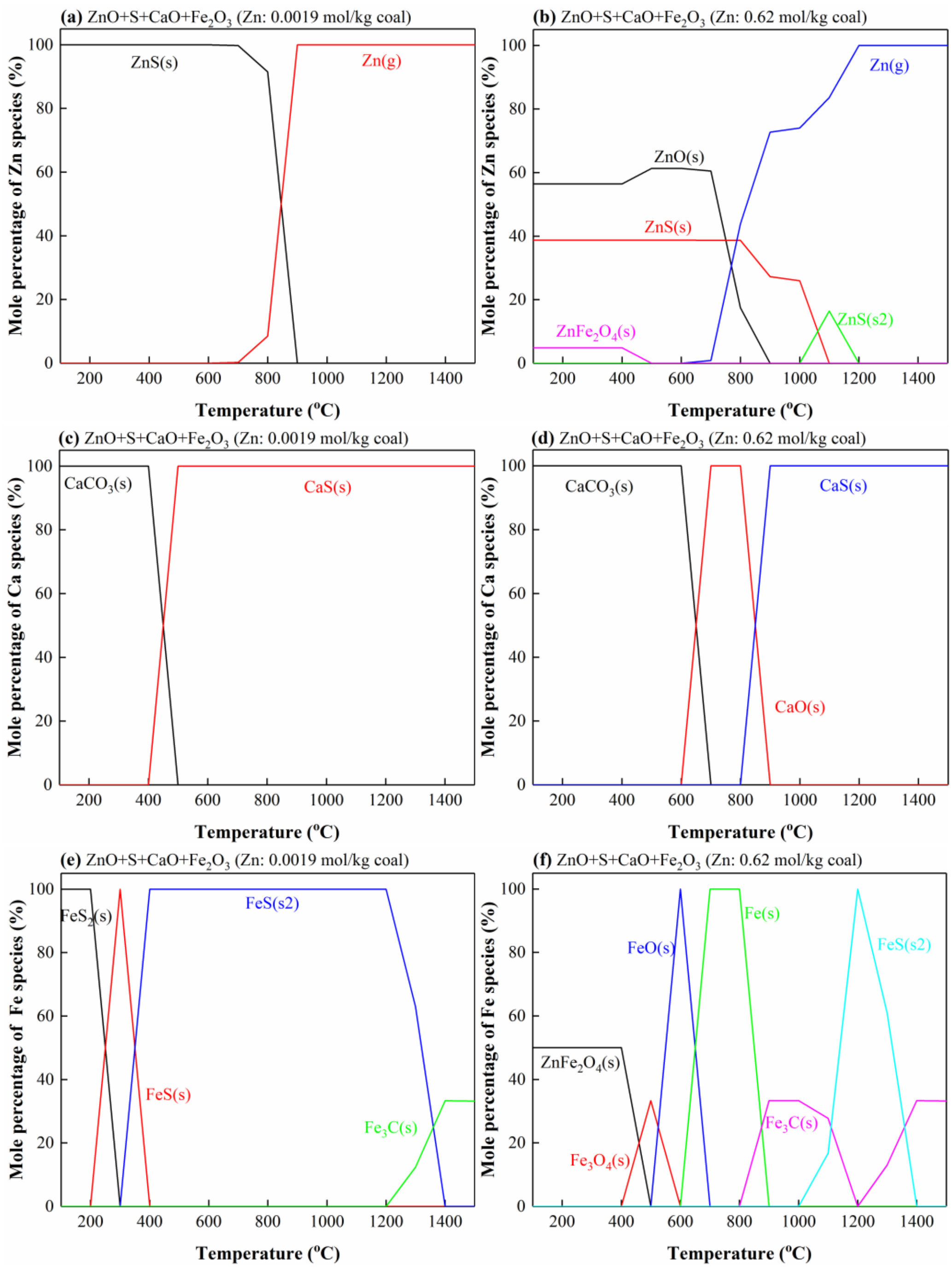

Figure S2. The thermodynamic equilibrium distributions of zinc (a, b), calcium (c, d) and iron (e, f) when sulfur, zinc, calcium and iron coexist in the system.

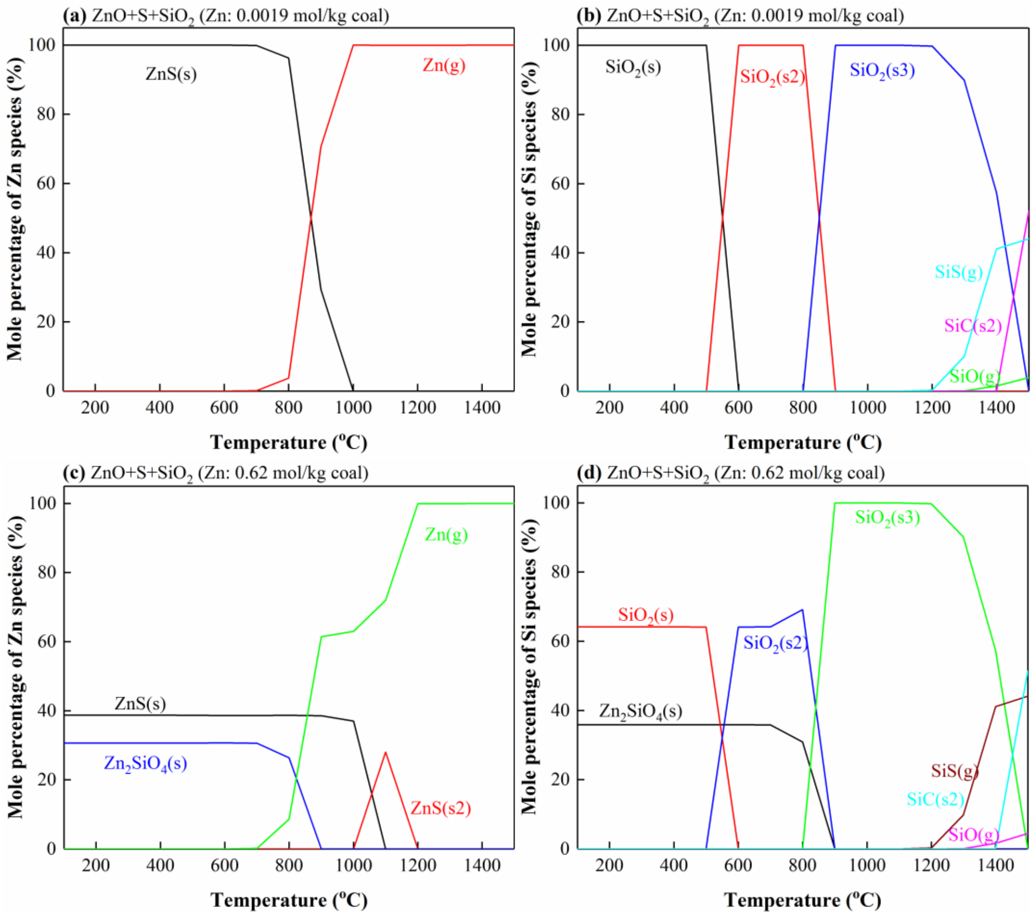

Figure S3. The thermodynamic equilibrium distributions of zinc (a, c) and silicon (b, d) when sulfur, zinc and silicon coexist in the system.

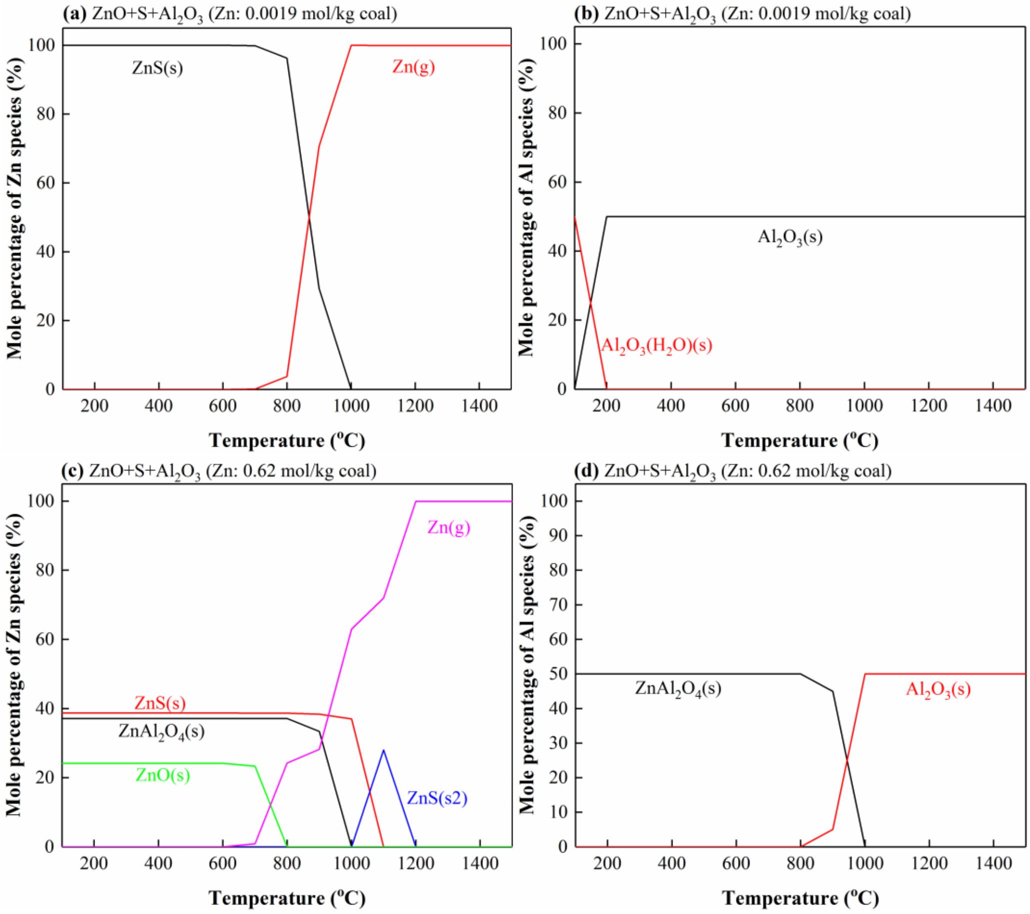

Figure S4. The thermodynamic equilibrium distributions of zinc (a, c) and aluminum (b, d) when sulfur, zinc and aluminum coexist in the system.

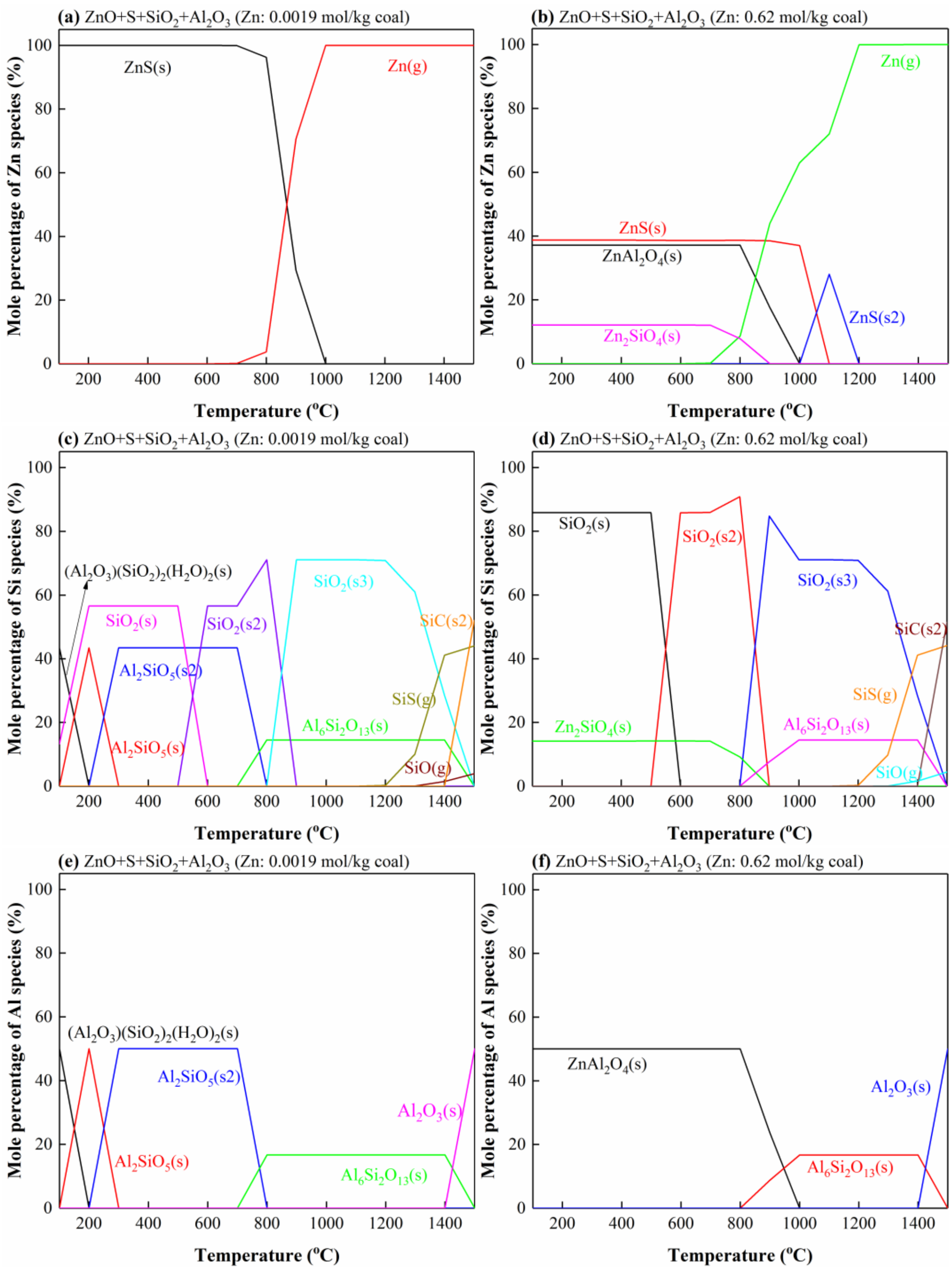

Figure S5. Thermodynamic equilibrium distributions of zinc (a, b), silicon (c, d) and aluminum (e, f) when sulfur, zinc, silicon and aluminum coexist in the system.

Table S2. Standard Gibbs free energies of typical reactions.

Reactions	The standard-state Gibbs free energy varied with temperature
$ZnO+C \rightarrow Zn(g)+CO(g)$ (1)	$\Delta_r G_m^\theta$ = 281454.29-294.35 t (100-1500 °C)
$CaO+ZnS+C \rightarrow CaS+Zn(g)+CO(g)$ (2)	$\Delta_r G_m^\theta$ = 294978.77-294.86 t (100-1500 °C)
$ZnO+Fe_2O_3 \rightarrow ZnFe_2O_4$ (3)	$\Delta_r G_m^\theta$ = -3858.45-10.17 t (100-600 °C)
	$\Delta_r G_m^\theta$ = -11292.38+2.5442 t (700-1500 °C)
$2ZnO+SiO_2 \rightarrow Zn_2SiO_4$ (4)	$\Delta_r G_m^\theta$ = -33008.05+6.12 t (100-1500 °C)
$Zn_2SiO_4+2C \rightarrow SiO_2+2Zn(g)+2CO(g)$ (5)	$\Delta_r G_m^\theta$ = 595916.63-594.82 t (100-1500 °C)
$SiO_2+C \rightarrow SiO(g)+CO(g)$ (6)	$\Delta_r G_m^\theta$ = 594968.48-343.75 t (100-1500 °C)
$SiO_2+3C \rightarrow SiC+2CO(g)$ (7)	$\Delta_r G_m^\theta$ = 515358.30-342.19 t (100-1500 °C)
$SiO_2+S+2C \rightarrow SiS(g)+2CO(g)$ (8)	$\Delta_r G_m^\theta$ = 638087.82-491.71 t (100-1500 °C)
$ZnO+Al_2O_3 \rightarrow ZnAl_2O_4$ (9)	$\Delta_r G_m^\theta$ = -43183.7+6.60 t (100-1500 °C)
$ZnAl_2O_4+C \rightarrow Al_2O_3+Zn(g)+CO(g)$ (10)	$\Delta_r G_m^\theta$ = 324638-300.92 t (100-1500 °C)
$3Al_2SiO_5 \rightarrow Al_6Si_2O_{13}+SiO_2$ (11)	$\Delta_r G_m^\theta$ = 32981.22-40.17 t (100-1500 °C)
$Al_6Si_2O_{13}+6C \rightarrow 3Al_2O_3+2SiC+4CO(g)$ (12)	$\Delta_r G_m^\theta$ = 1015057.38-653.98 t (100-1500 °C)
$3ZnAl_2O_4+2SiO_2+3C \rightarrow Al_6Si_2O_{13}+3Zn(g)+3CO(g)$ (13)	$\Delta_r G_m^\theta$ = 989573.27-933.14 t (100-1500 °C)

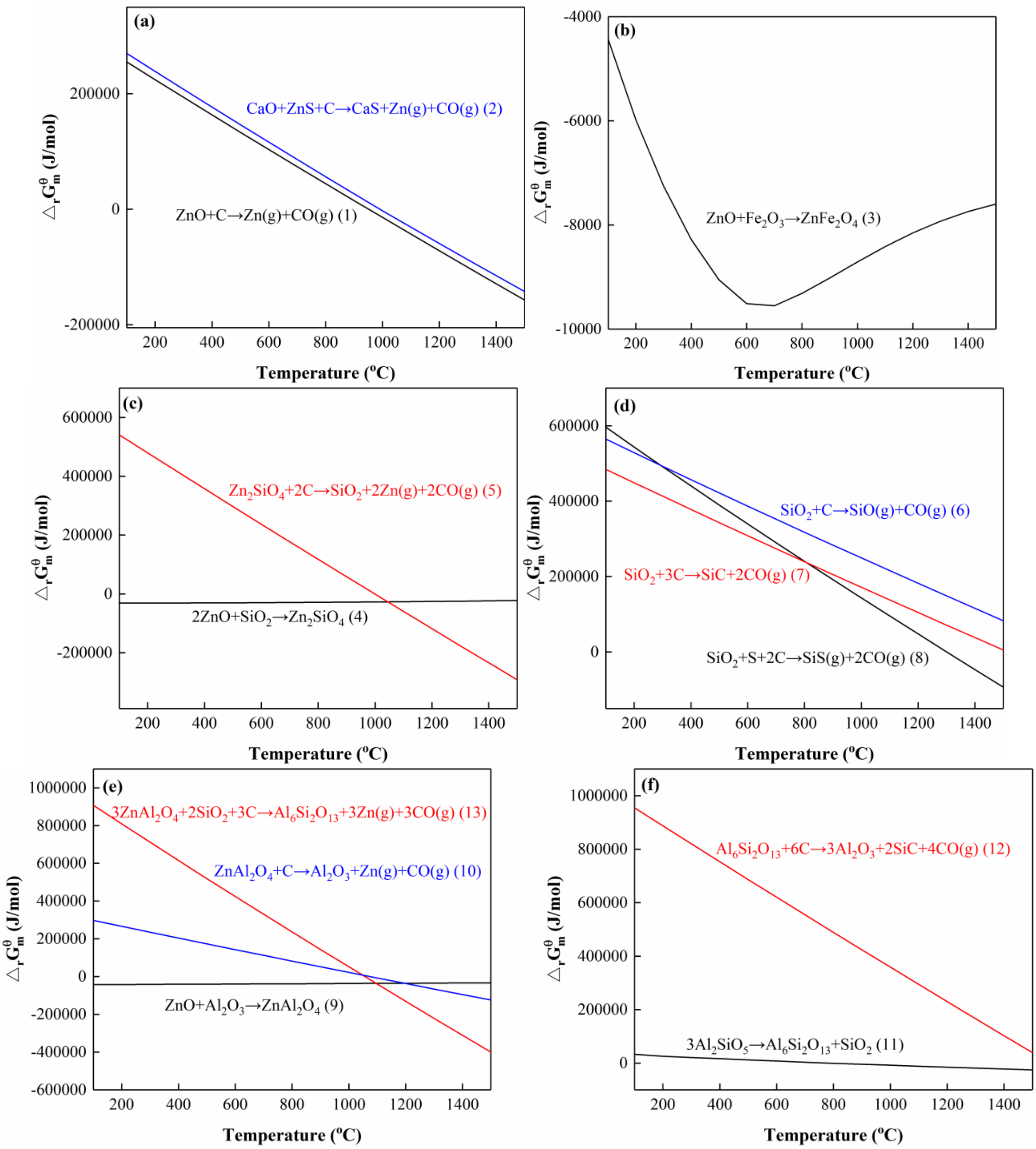

Figure S6. The standard-state Gibbs free energies of reactions 1-13 as a function of tempera ture.

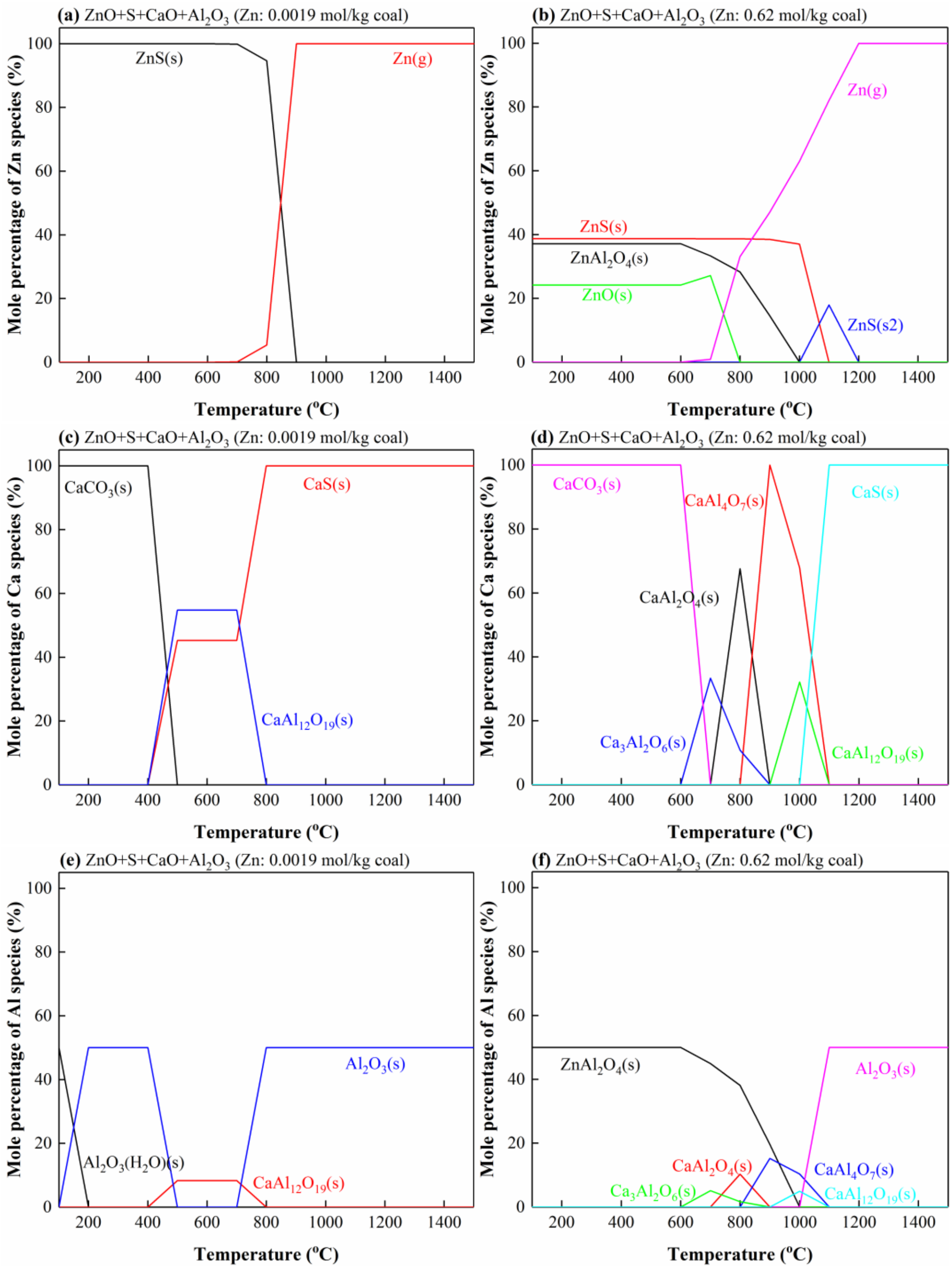

Figure S7. Thermodynamic equilibrium distributions of zinc (a, b), calcium (c, d) and aluminum (e, f) when sulfur, zinc, calcium and aluminum coexist in the system.

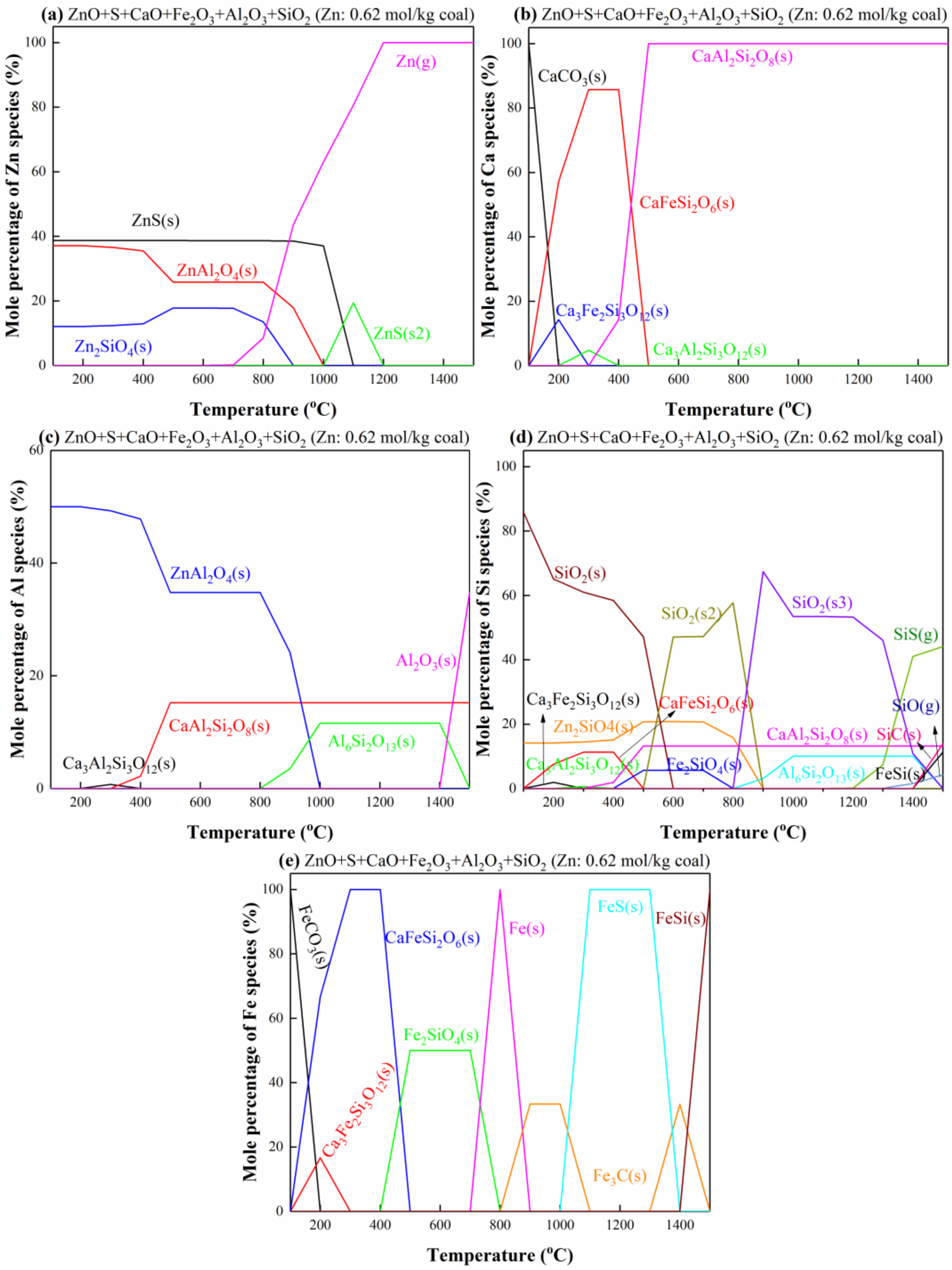

Figure S8. Thermodynamic equilibrium distributions of Zn (a), Ca (b), Al (c), Si (d) and Fe (e) in the coal when the Zn content is high (Zn/S/Ca/Al/Si/Fe =0.62/0.24/0.07/0.46/0.53/0.06).