Electronic Supplemental Information

CO_2 conversion to CO by reverse water gas shift and dry reforming using chemical looping

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Calculation details for the modified Ellingham diagrams

Heat capacity, enthalpy, and entropy for some simple oxide and metal used values are listed by the National Institute of Standards and Technology (NIST) [1]. Materials using NIST's values are presented in Table S1. Helmholtz free energies of other materials, including composite oxides and alloys, were calculated using PFP [2] ver. 5.0.0 of Matlantis [3]. Here, the Gibbs energy of a material is considered equal to Helmholtz free energies of the material because of low contribution of work to Gibbs energy in the case of solids. Gibbs energies and Helmholtz free energies were obtained according to the following equation.

$$G(T,p) = H(T) - T \times S(T) + RT \times ln(\frac{p}{p^{\circ}}) \quad \text{(eq. S1)}$$

$$F(T) = U(T) - U(298.15) + U_{formation}(298.15) - T \times S(T) \quad \text{(eq. S2)}$$

Therein, G, H, T, S, R, p, p°, F, U, and $U_{formation}$ respectively represent the Gibbs energy, enthalpy, temperature, entropy, the gas constant, partial pressure of a target gas, 1 atm of standard pressure, Helmholtz free energy, internal energy, and formation internal energy.

PFP is a neural network potential constructed to reproduce the results of density functional theory (DFT) calculations, leading to fast phonon calculation. Actually, PFP is expected for accurate calculations for materials assessed in this review because of the large number of energies and forces of disordered binary crystal included in its training dataset. To overcome the electron localisation problem of metal oxides, a DFT+*U*-based mode of PFP was applied to the calculations of metal oxides, although a DFT-based mode of PFP was applied to the calculations of metals and alloys. Mixing results of DFT and DFT+*U* leads to inaccurate formation internal energy or enthalpy [4–6]. Based on a reported approach [6], the calculated internal energies were corrected by fitting between experimental formation enthalpies and calculated formation internal energies from mixing DFT and DFT+*U*. The experimental formation enthalpies are listed in Table S2. This method calculates the Gibbs energy of the crystal without considering the melting point. Therefore, some materials in the Ellingham diagrams have lines drawn to temperatures higher than the melting point.

All calculations were performed under a unified condition. All crystal structures were obtained from the Materials Project [7]. Structural optimisations with fixation of symmetry were first conducted. The optimiser was L-BFGS implemented in ASE [8]. The convergence criterion was 5 × 10^{-3} eV/ Å. Subsequently, internal energies and entropies were calculated through phonon calculations. The crystals were repeated until all lengths of cell edges were greater than 40 Å, the degree of displacement was 0.1 Å, and k-points were set as 20 × 20 × 20 on phonon calculations. The results of the phonon calculations were converted to the density of the state. Then they used for thermodynamics calculations of a periodic system of independent harmonic oscillators.

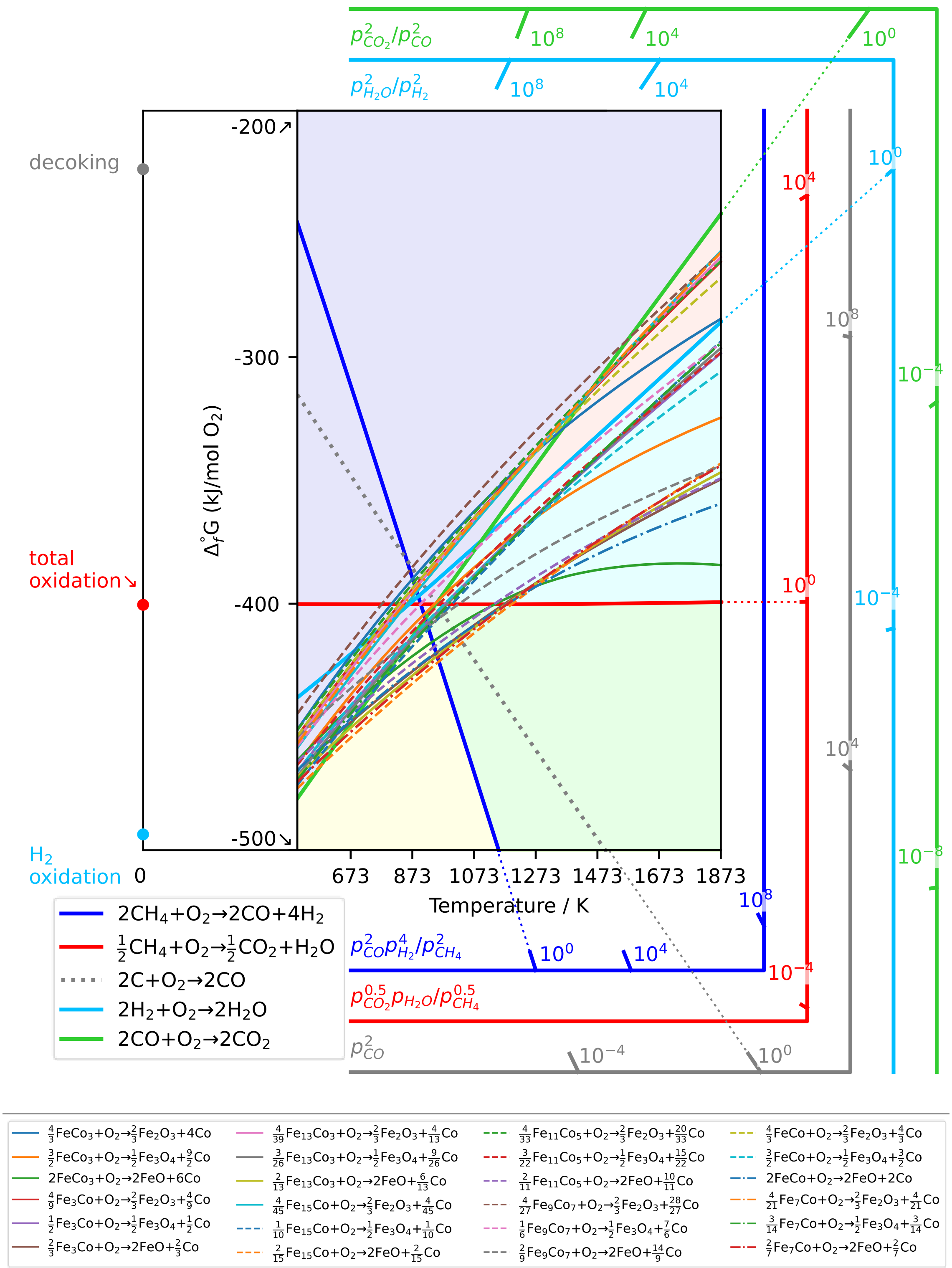

Fig. S1 Modified Ellingham diagram for Fe-Co alloy oxygen carriers during chemical looping.

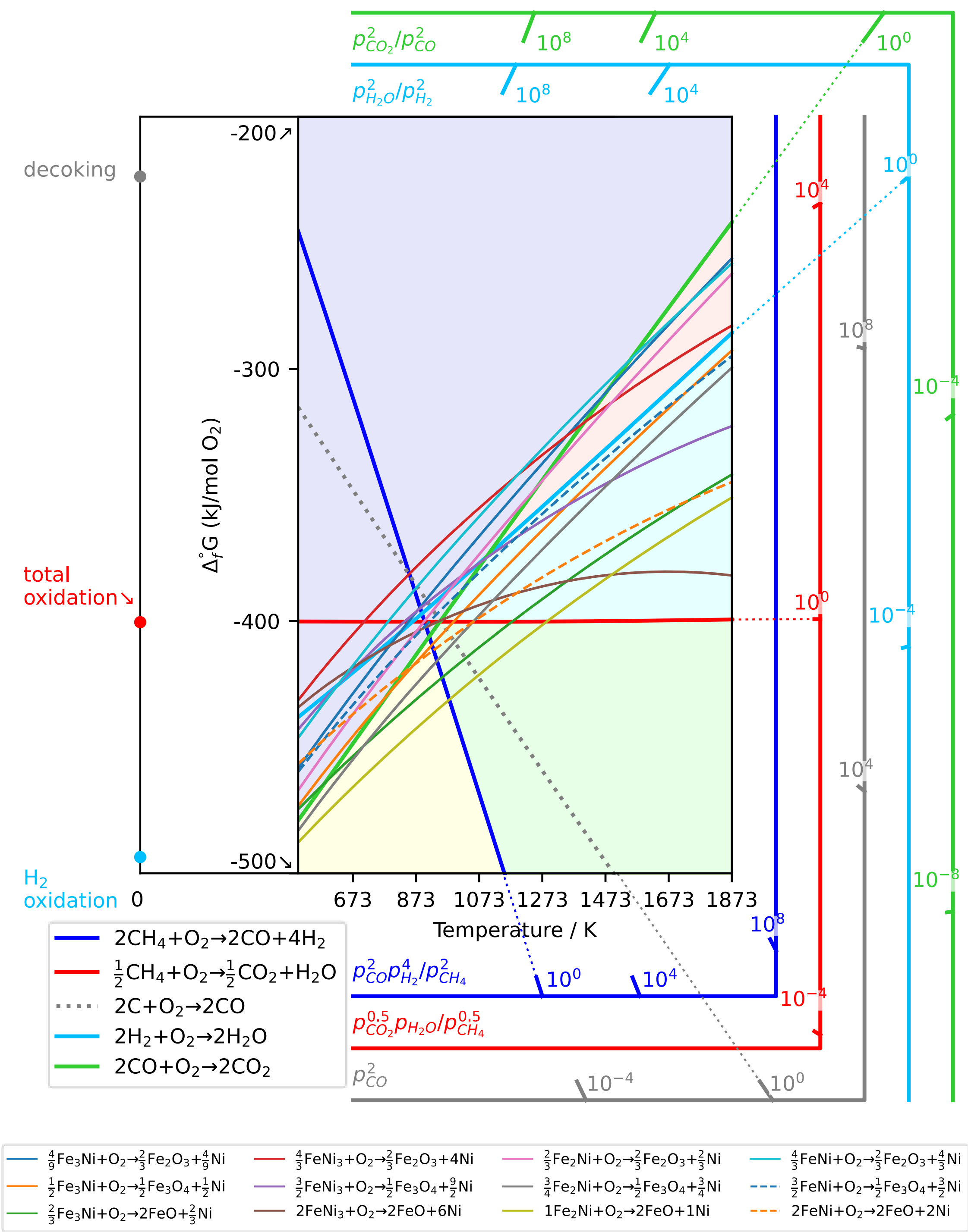

Fig. S2 Modified Ellingham diagram for Fe-Ni alloy oxygen carriers during chemical looping.

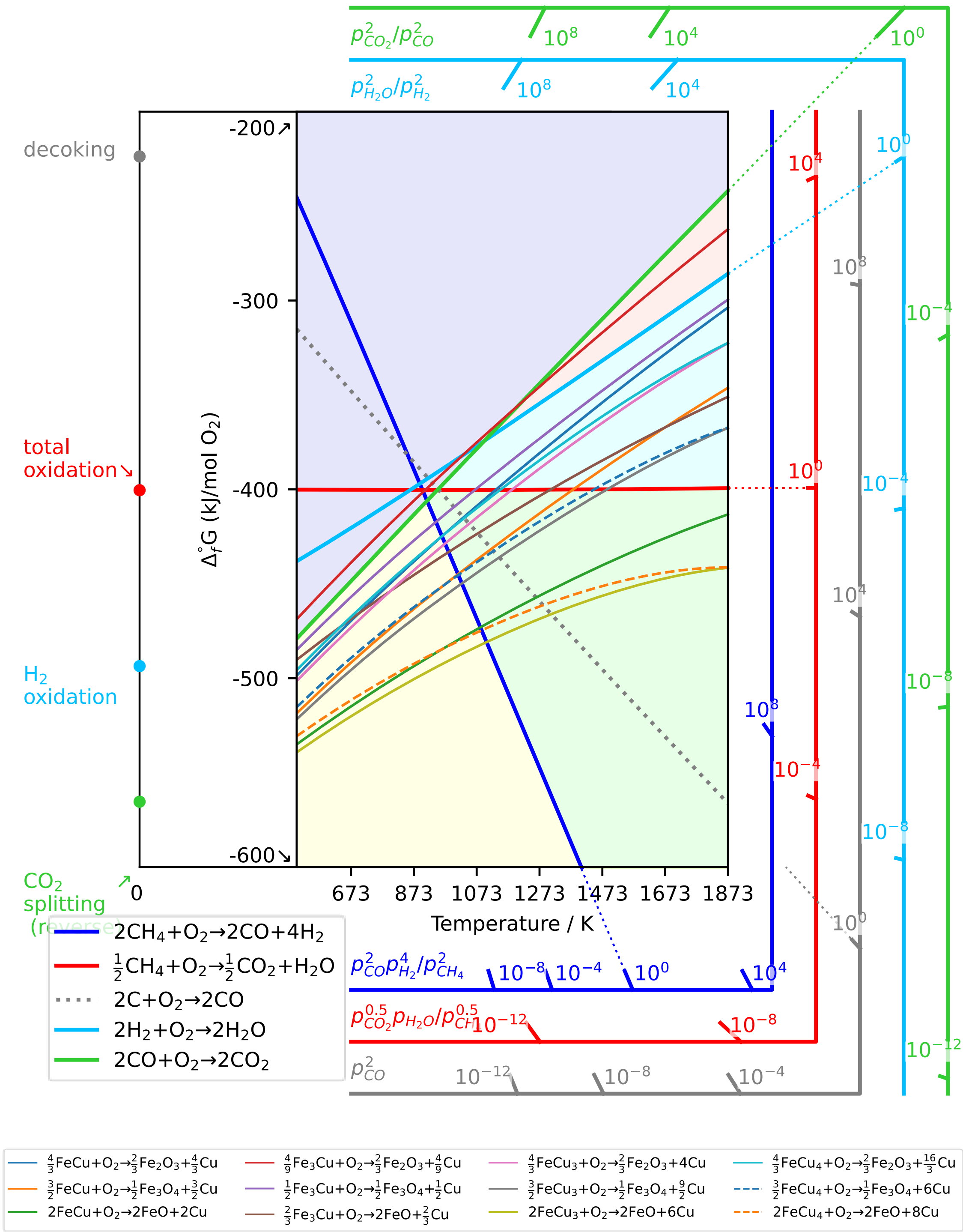

Fig. S3 Modified Ellingham diagram for Fe-Cu alloy oxygen carriers during chemical looping.

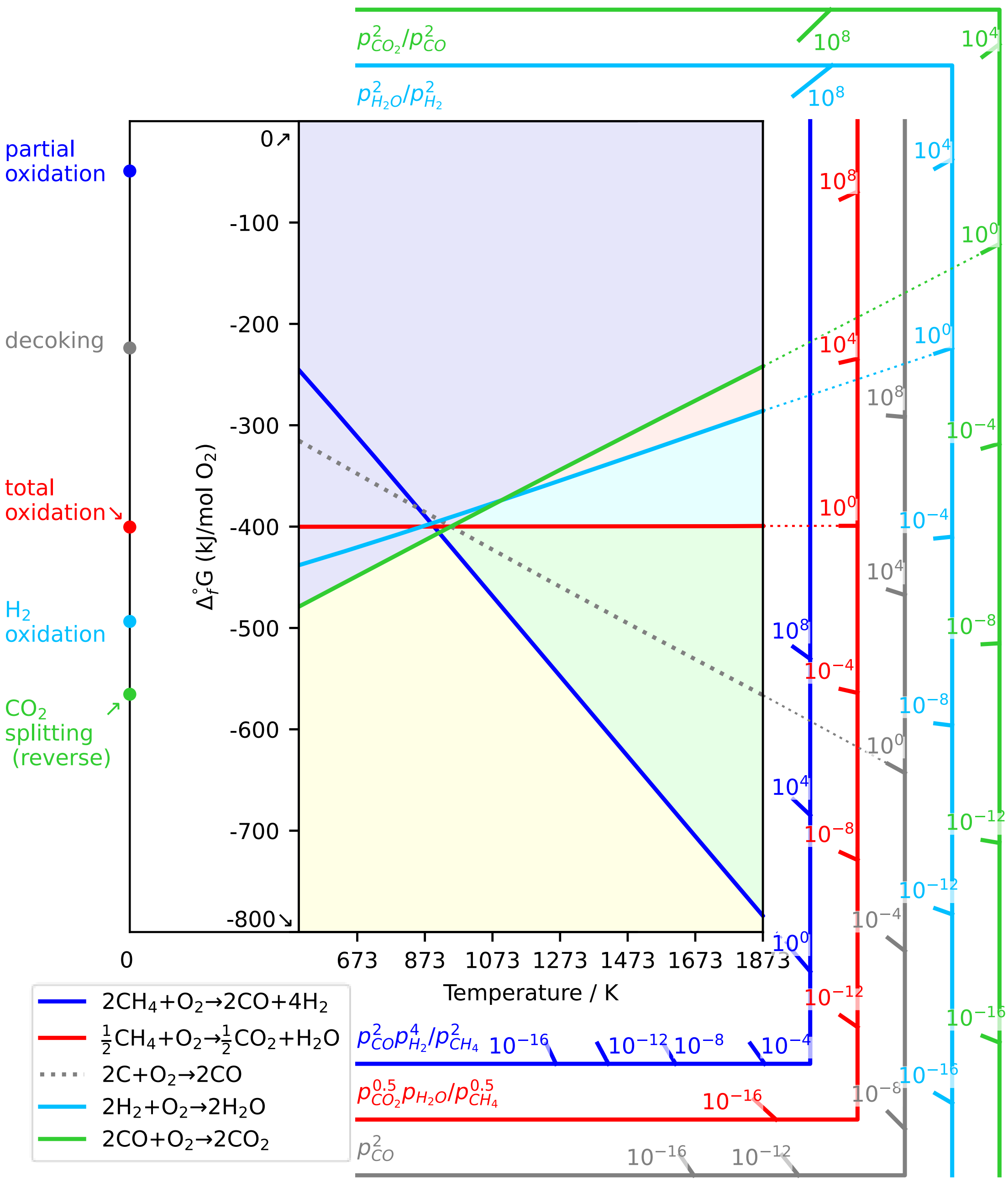

Fig. S4 Modified Ellingham diagram for Fe-Ru alloy oxygen carriers during chemical looping. There is no reaction within the drawing area.

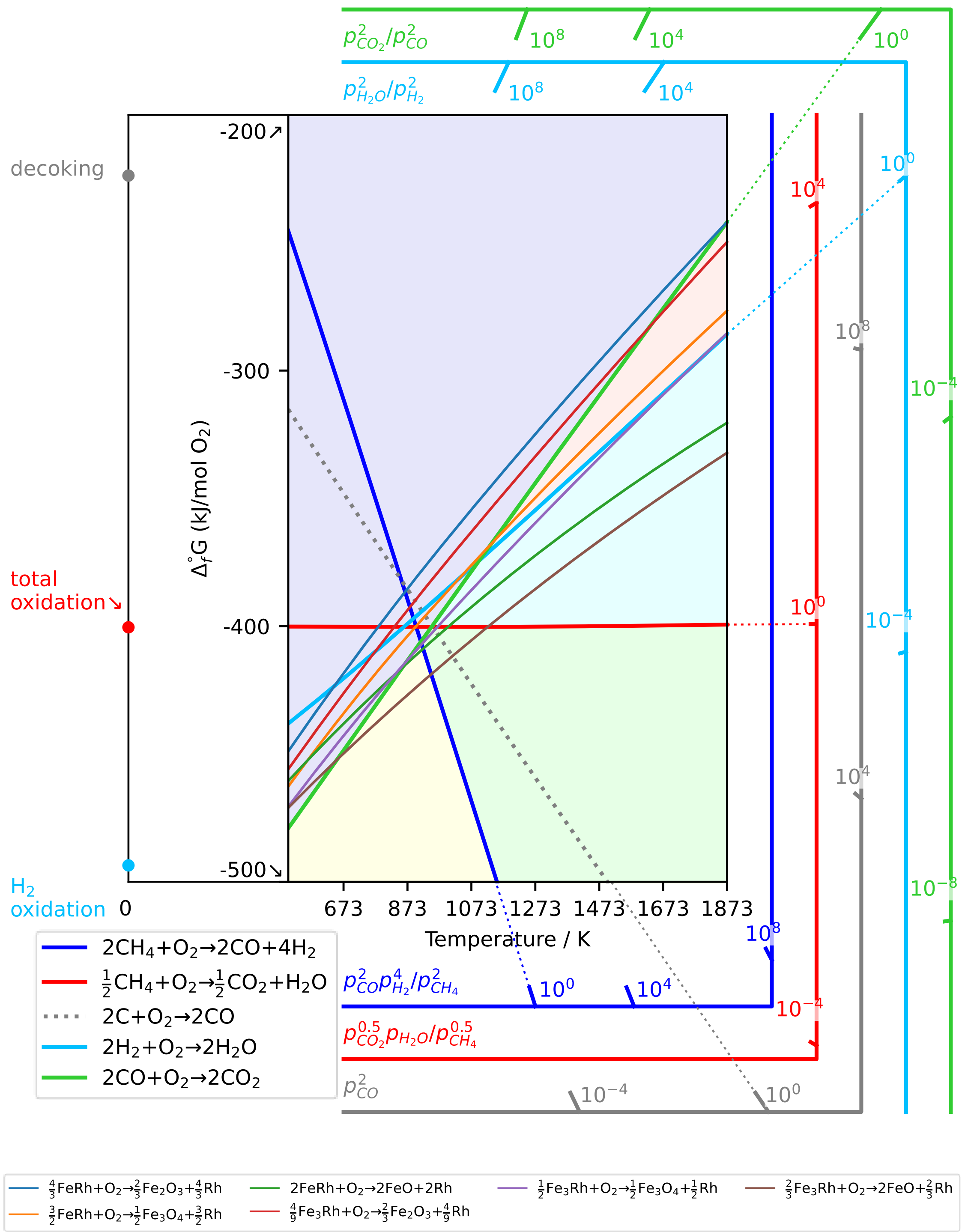

Fig. S5 Modified Ellingham diagram for Fe-Rh alloy oxygen carriers during chemical looping.

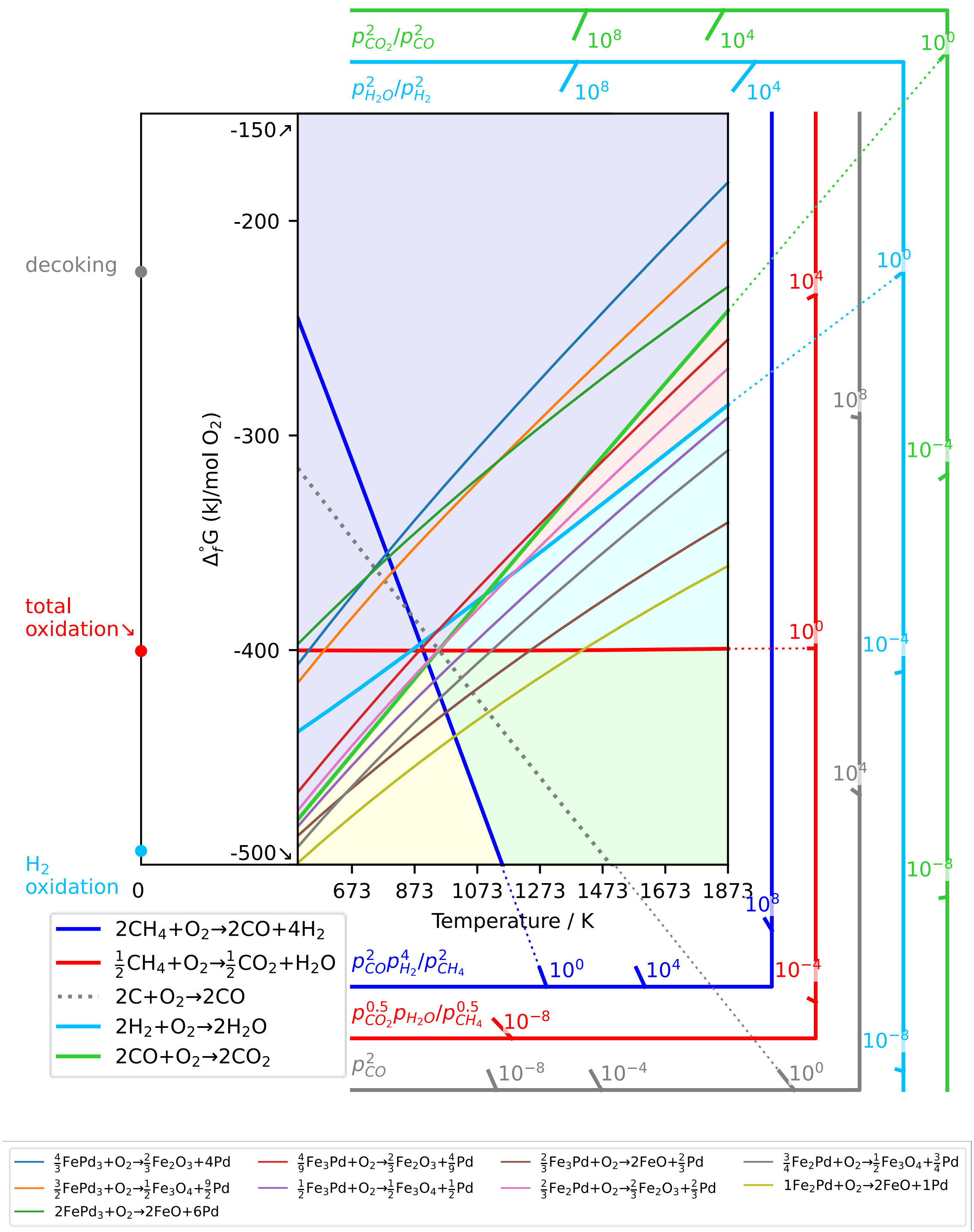

Fig. S6 Modified Ellingham diagram for Fe-Pd alloy oxygen carriers during chemical looping.

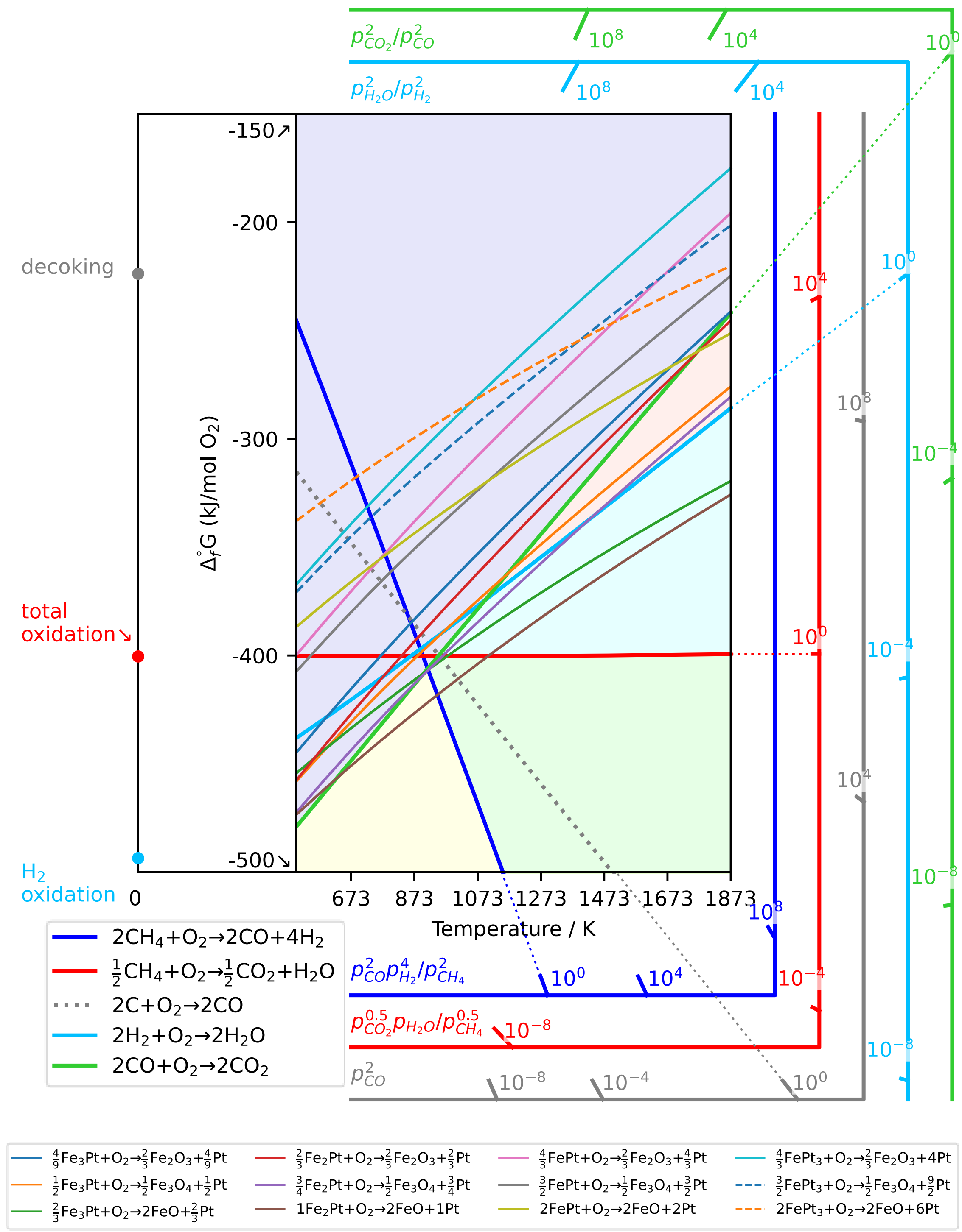

Fig. S7 Modified Ellingham diagram for Fe-Pt alloy oxygen carriers during chemical looping.

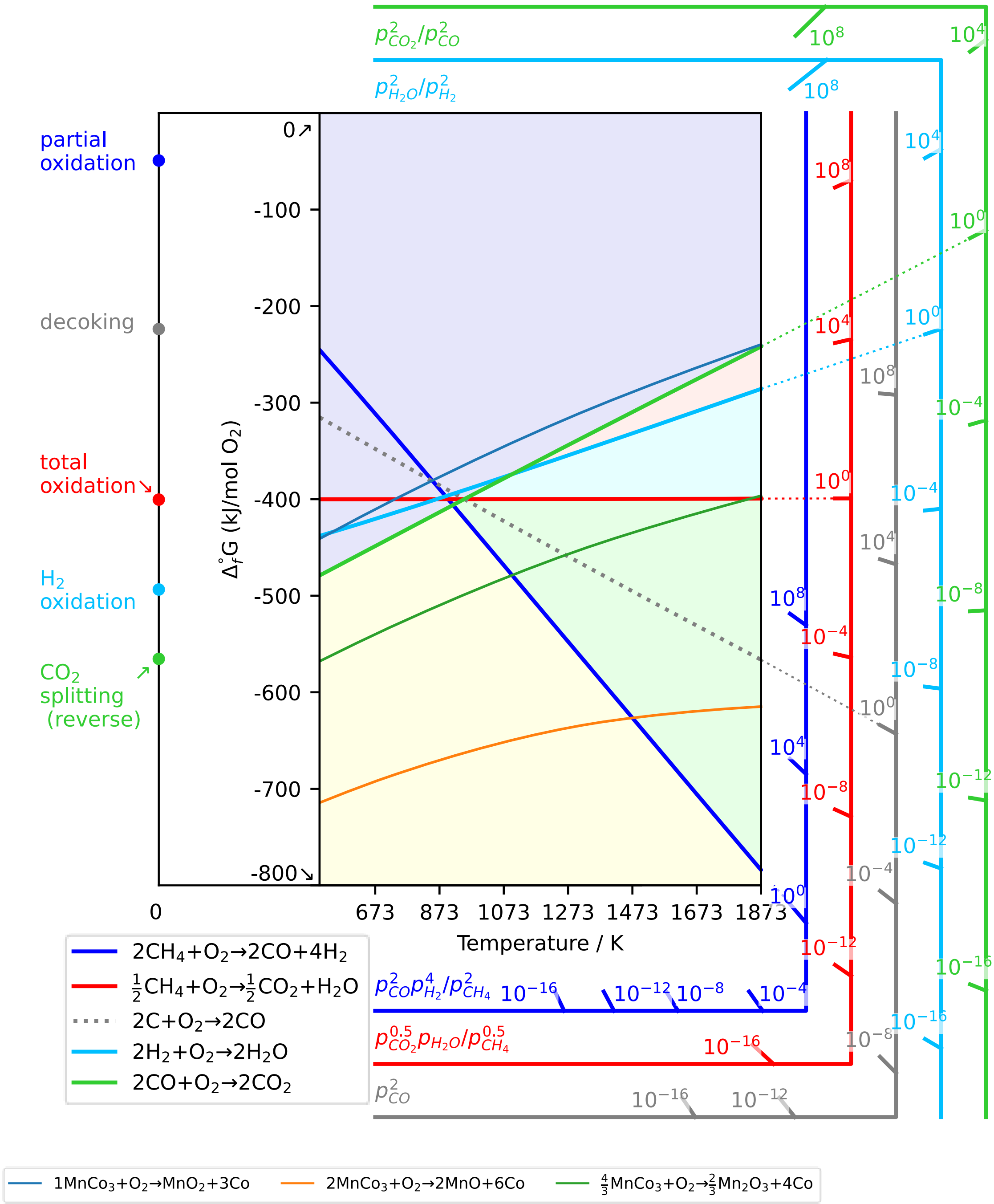

Fig. S8 Modified Ellingham diagram for Mn-Co alloy oxygen carriers during chemical looping.

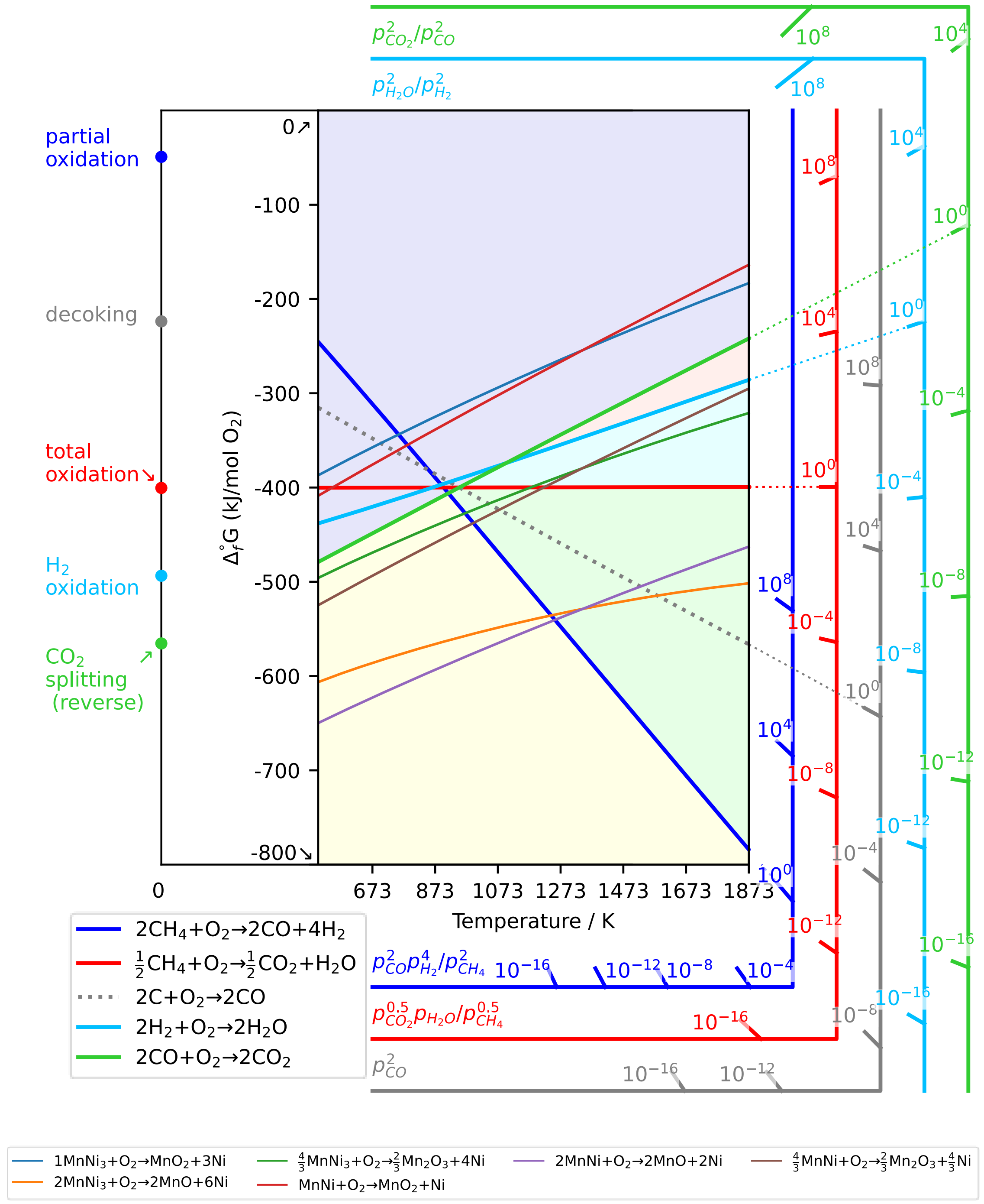

Fig. S9 Modified Ellingham diagram for Mn-Ni alloy oxygen carriers during chemical looping.

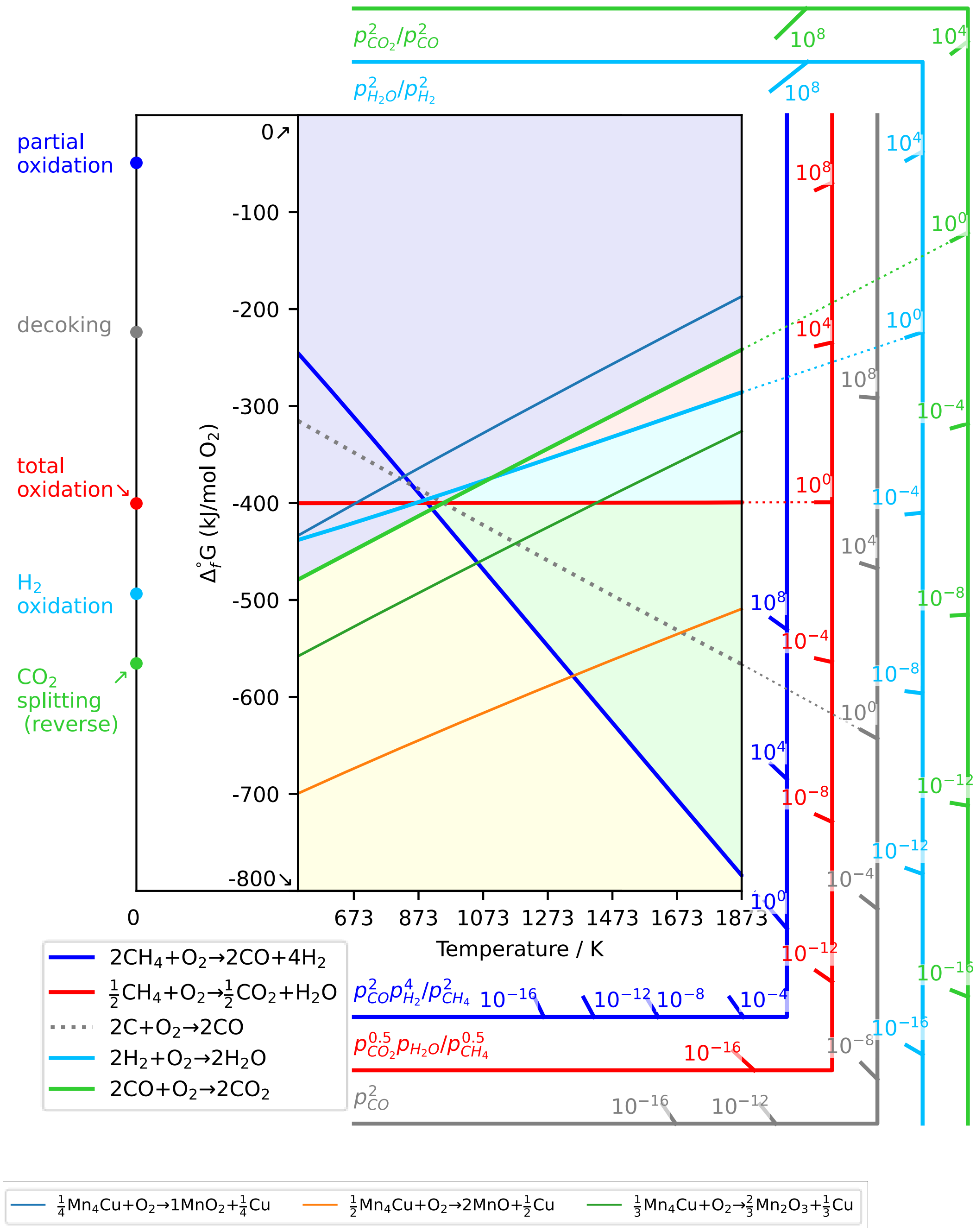

Fig. S10 Modified Ellingham diagram for Mn-Cu alloy oxygen carriers during chemical looping.

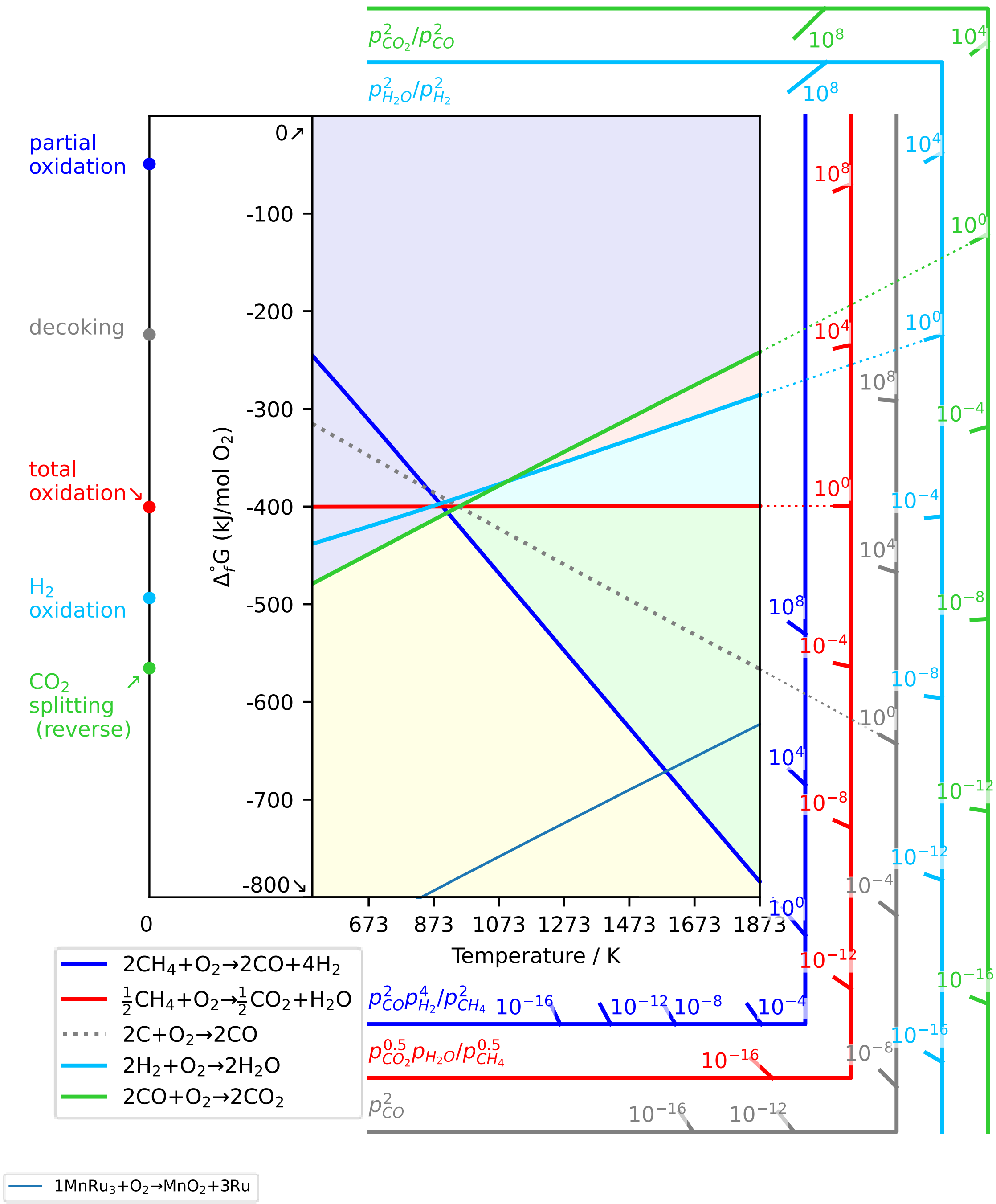

Fig. S11 Modified Ellingham diagram for Mn-Ru alloy oxygen carriers during chemical looping.

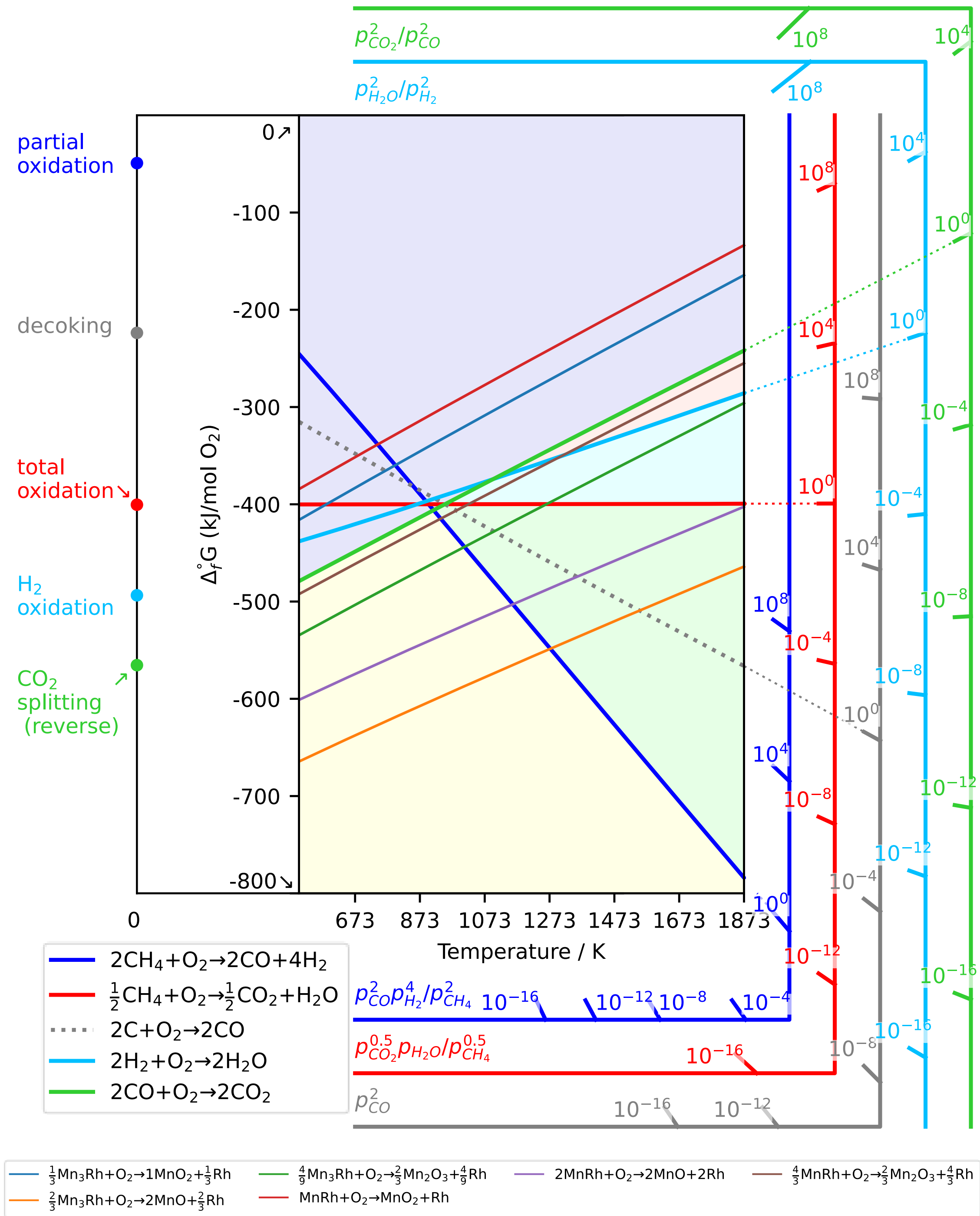

Fig. S12 Modified Ellingham diagram for Mn-Rh alloy oxygen carriers during chemical looping.

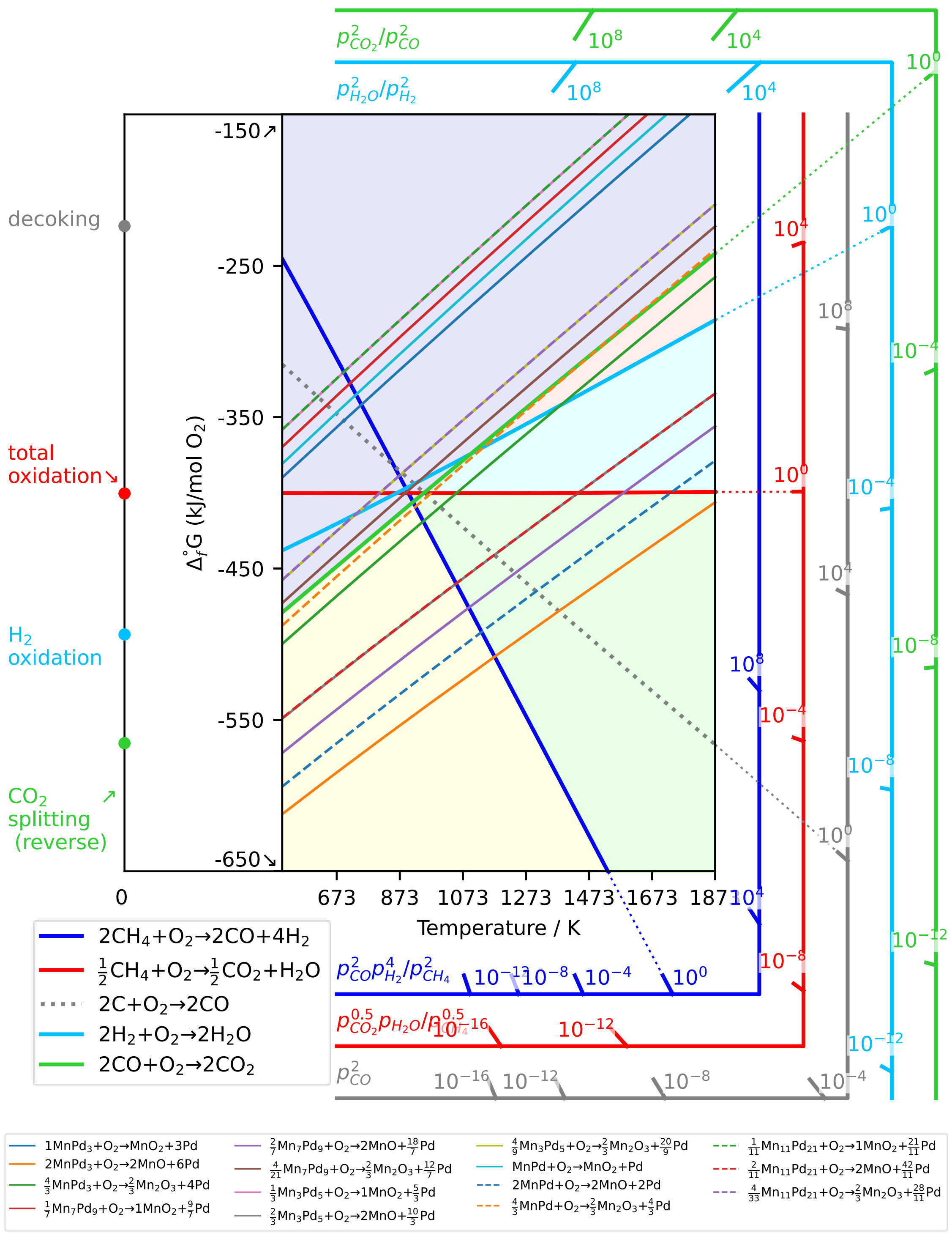

Fig. S13 Modified Ellingham diagram for Mn-Pd alloy oxygen carriers during chemical looping.

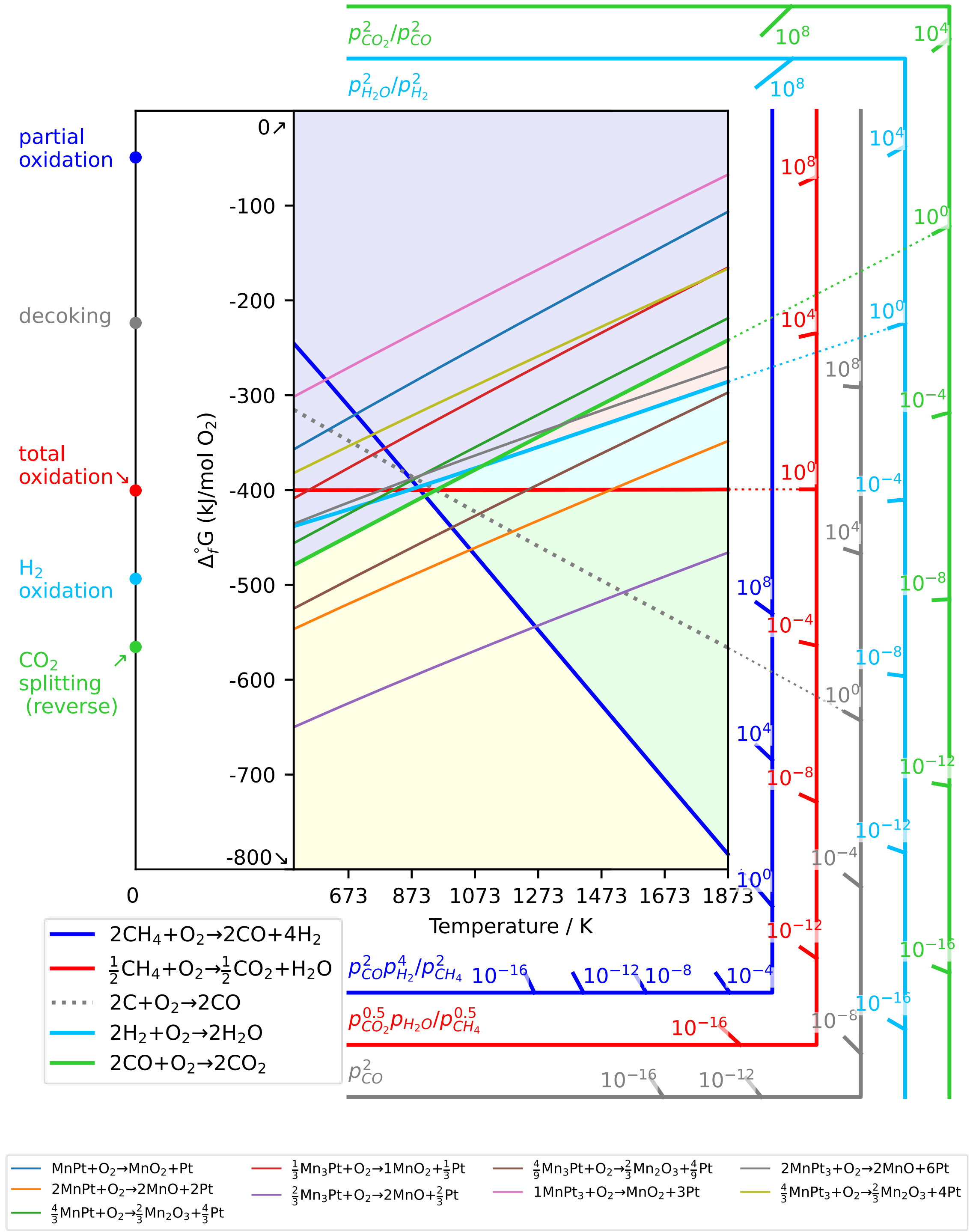

Fig. S14 Modified Ellingham diagram for Mn-Pt alloy oxygen carriers during chemical looping.

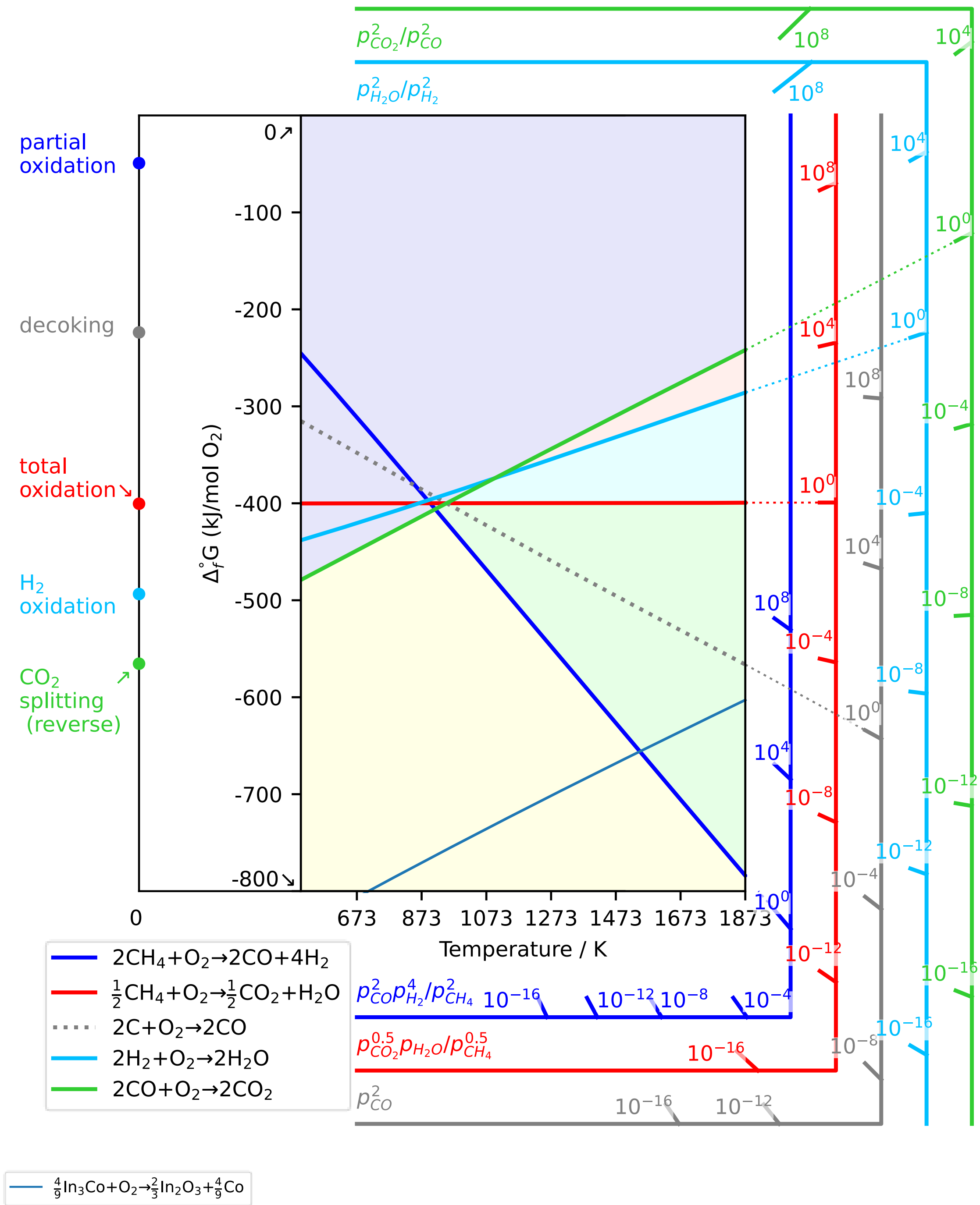

Fig. S15 Modified Ellingham diagram for In-Co alloy oxygen carriers during chemical looping.

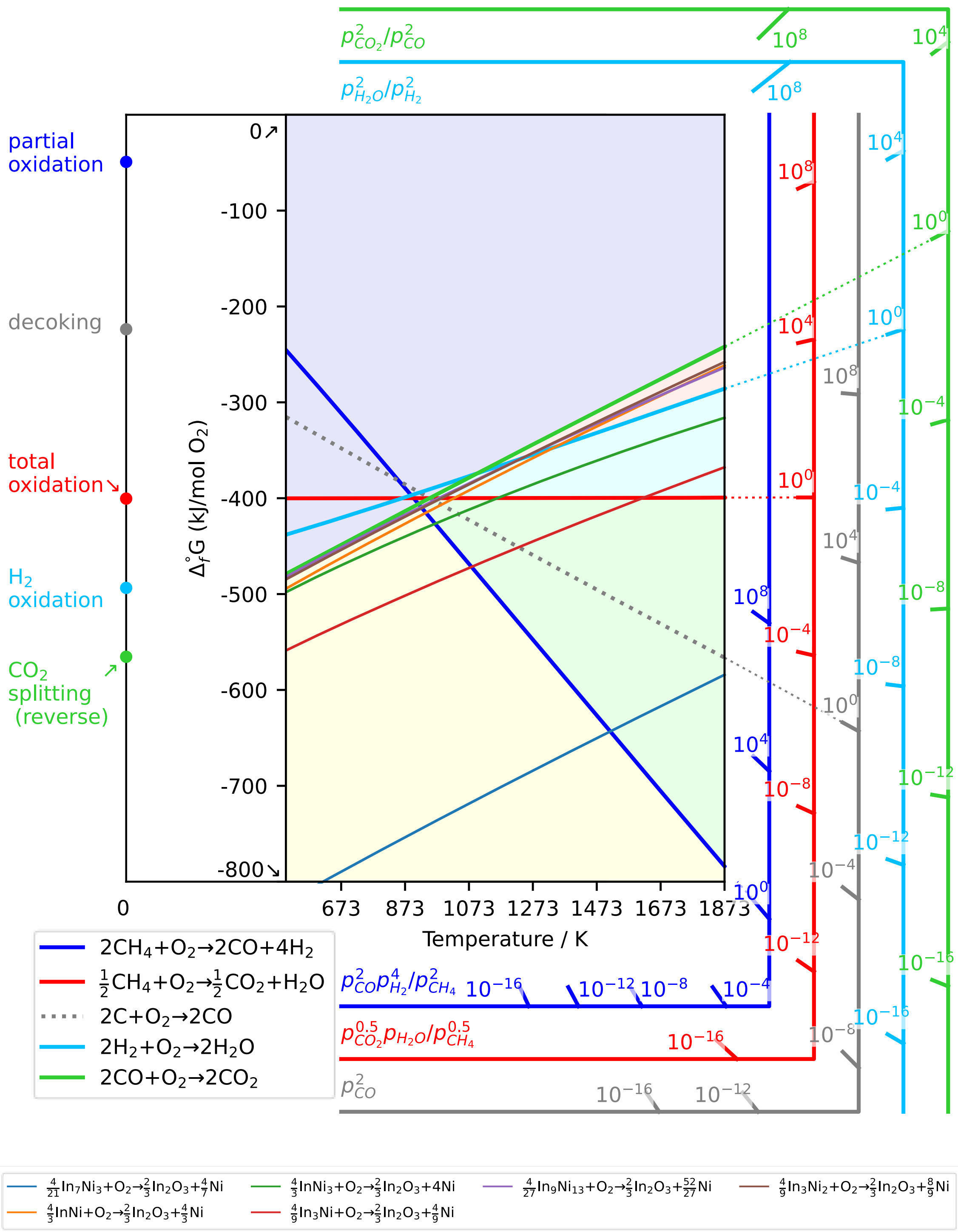

Fig. S16 Modified Ellingham diagram for In-Ni alloy oxygen carriers during chemical looping.

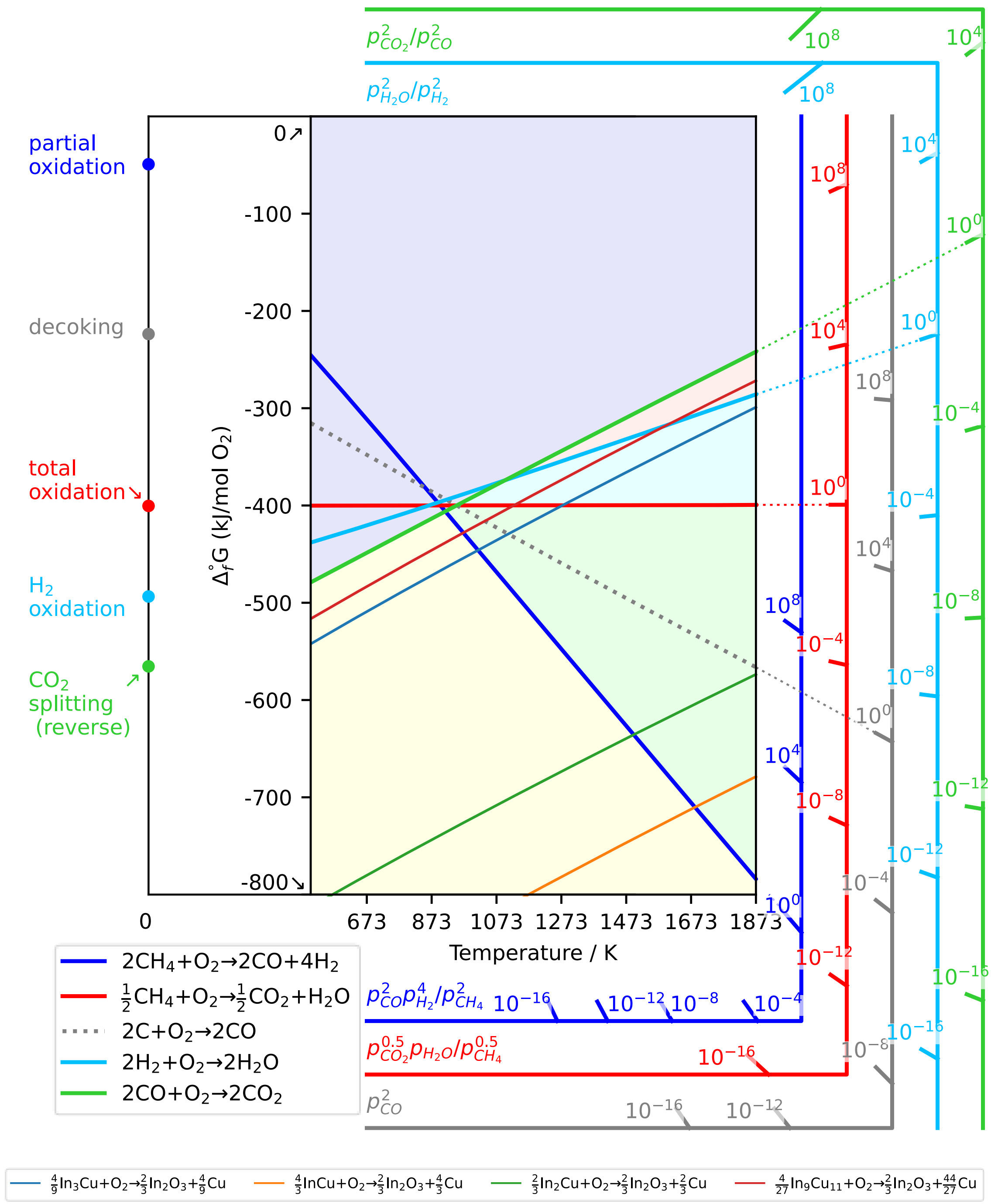

Fig. S17 Modified Ellingham diagram for In-Cu alloy oxygen carriers during chemical looping.

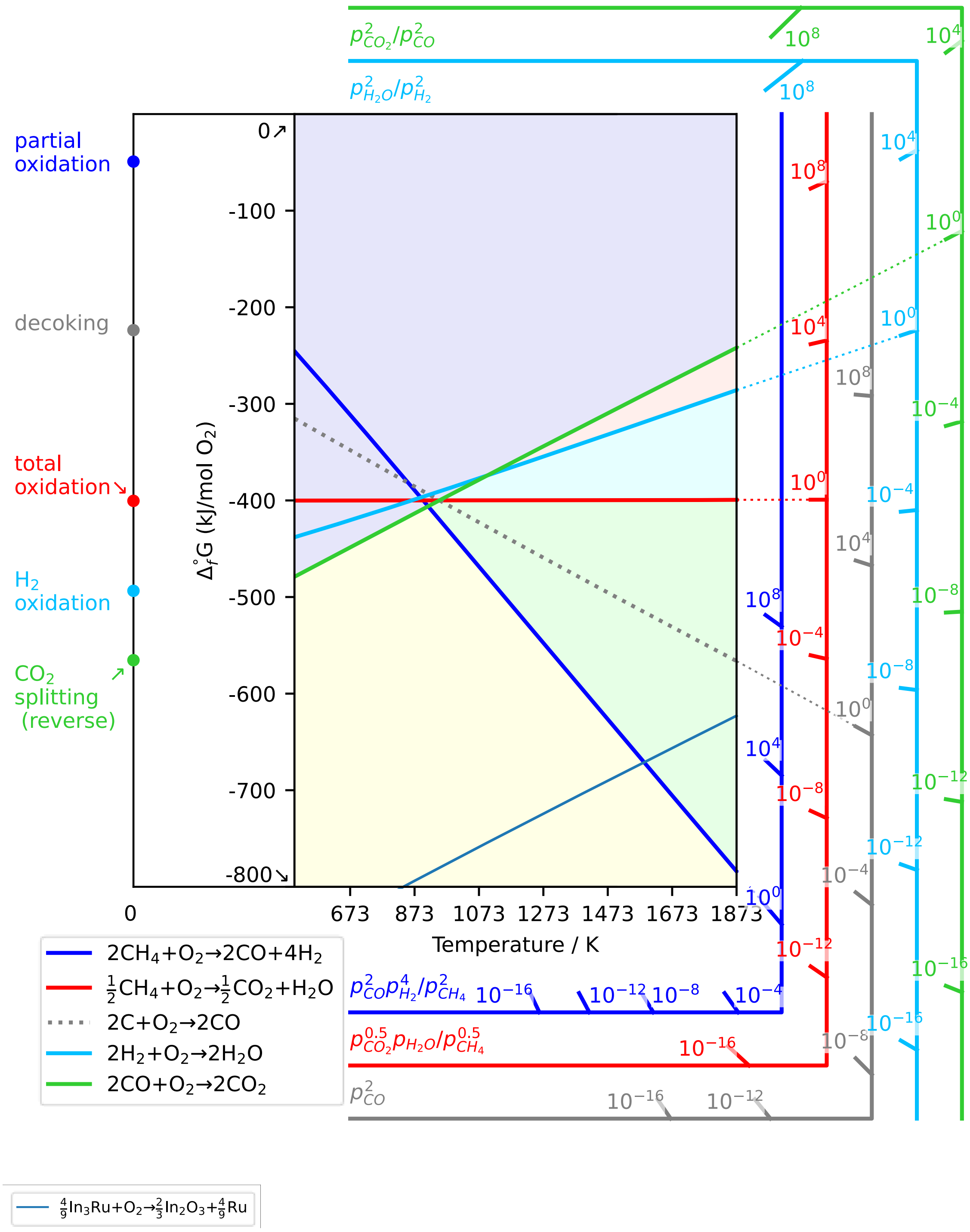

Fig. S18 Modified Ellingham diagram for In-Ru alloy oxygen carriers during chemical looping.

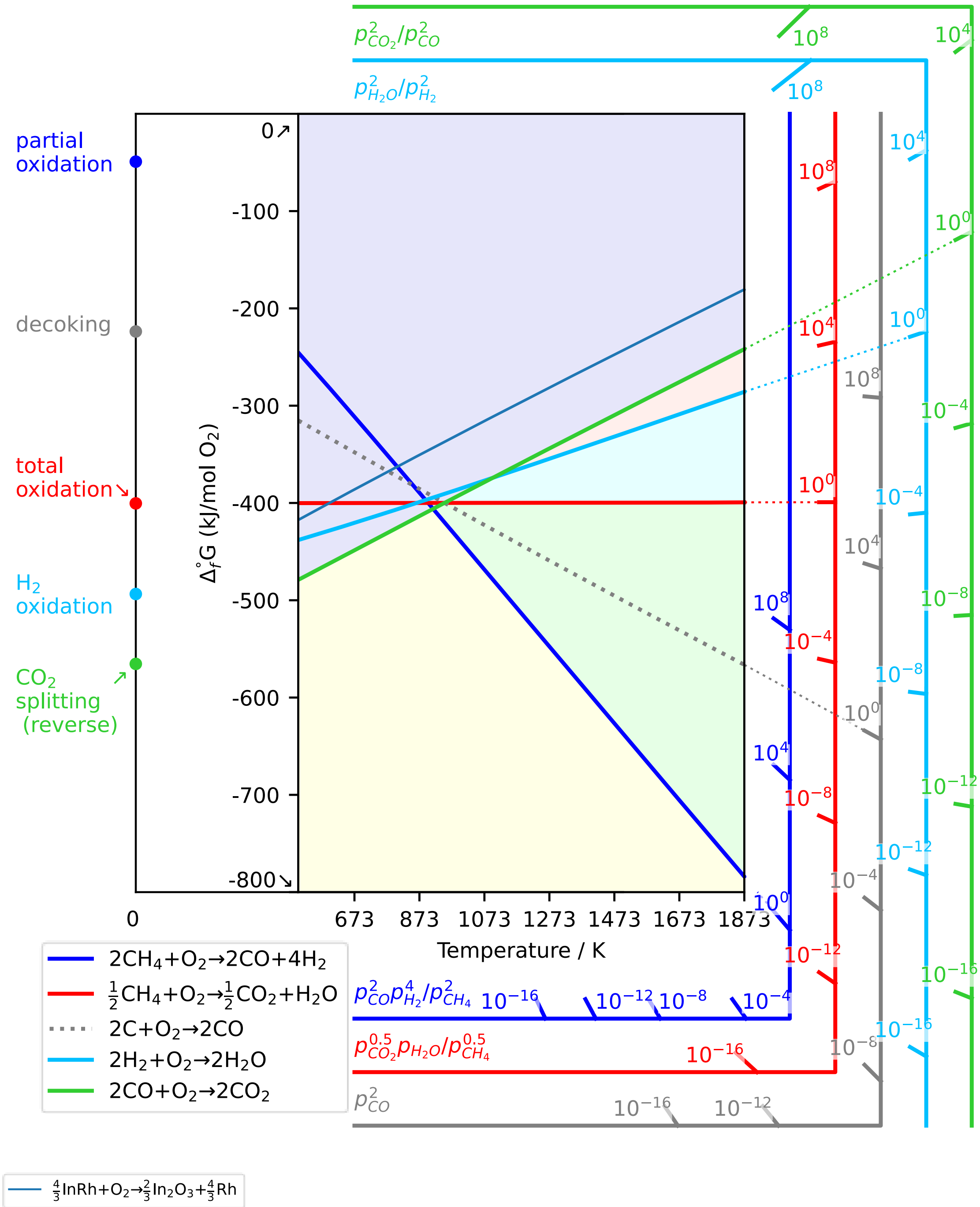

Fig. S19 Modified Ellingham diagram for In-Rh alloy oxygen carriers during chemical looping.

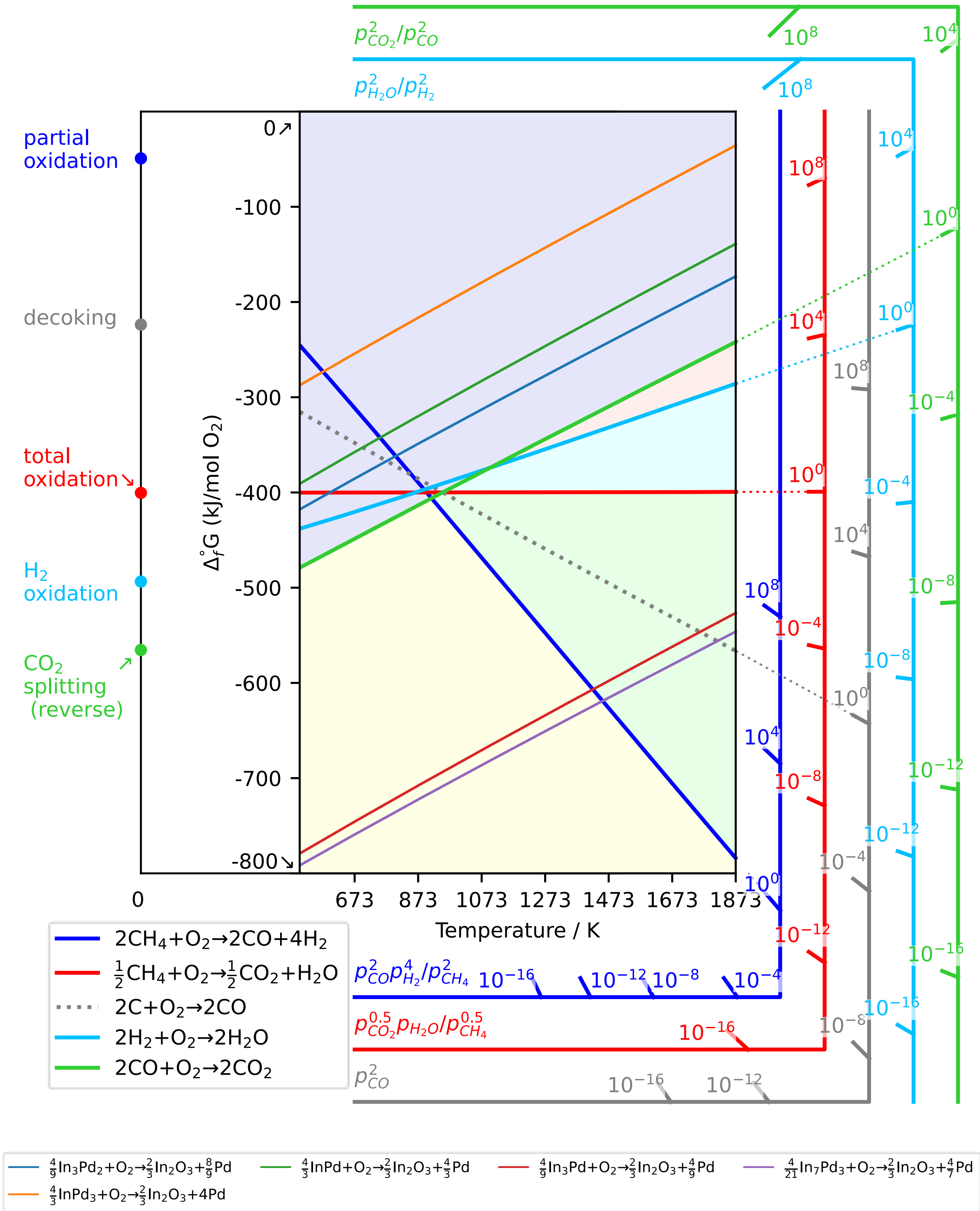

Fig. S20 Modified Ellingham diagram for In-Pd alloy oxygen carriers during chemical looping.

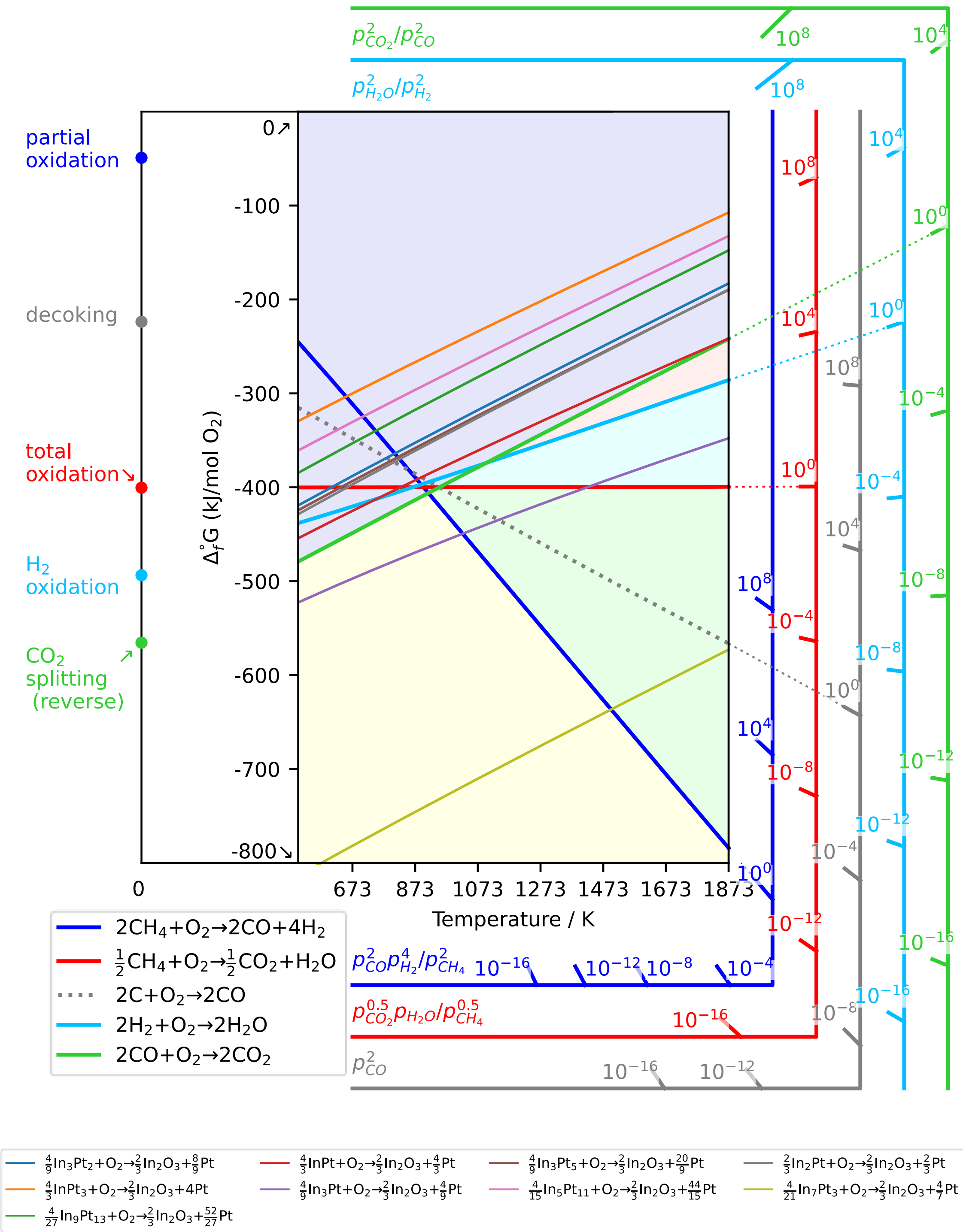

Fig. S21 Modified Ellingham diagram for In-Pt alloy oxygen carriers during chemical looping.

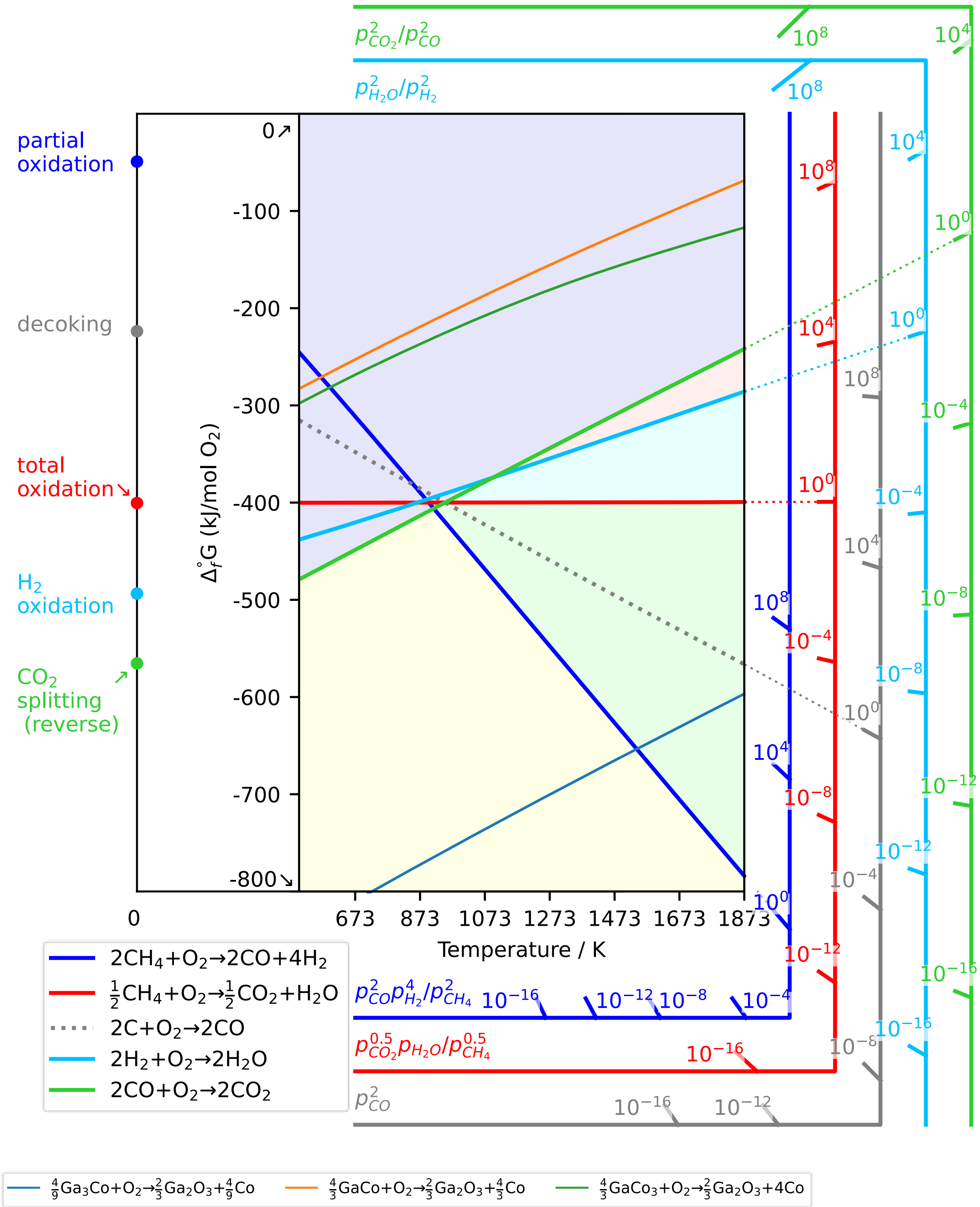

Fig. S22 Modified Ellingham diagram for Ga-Co alloy oxygen carriers during chemical looping.

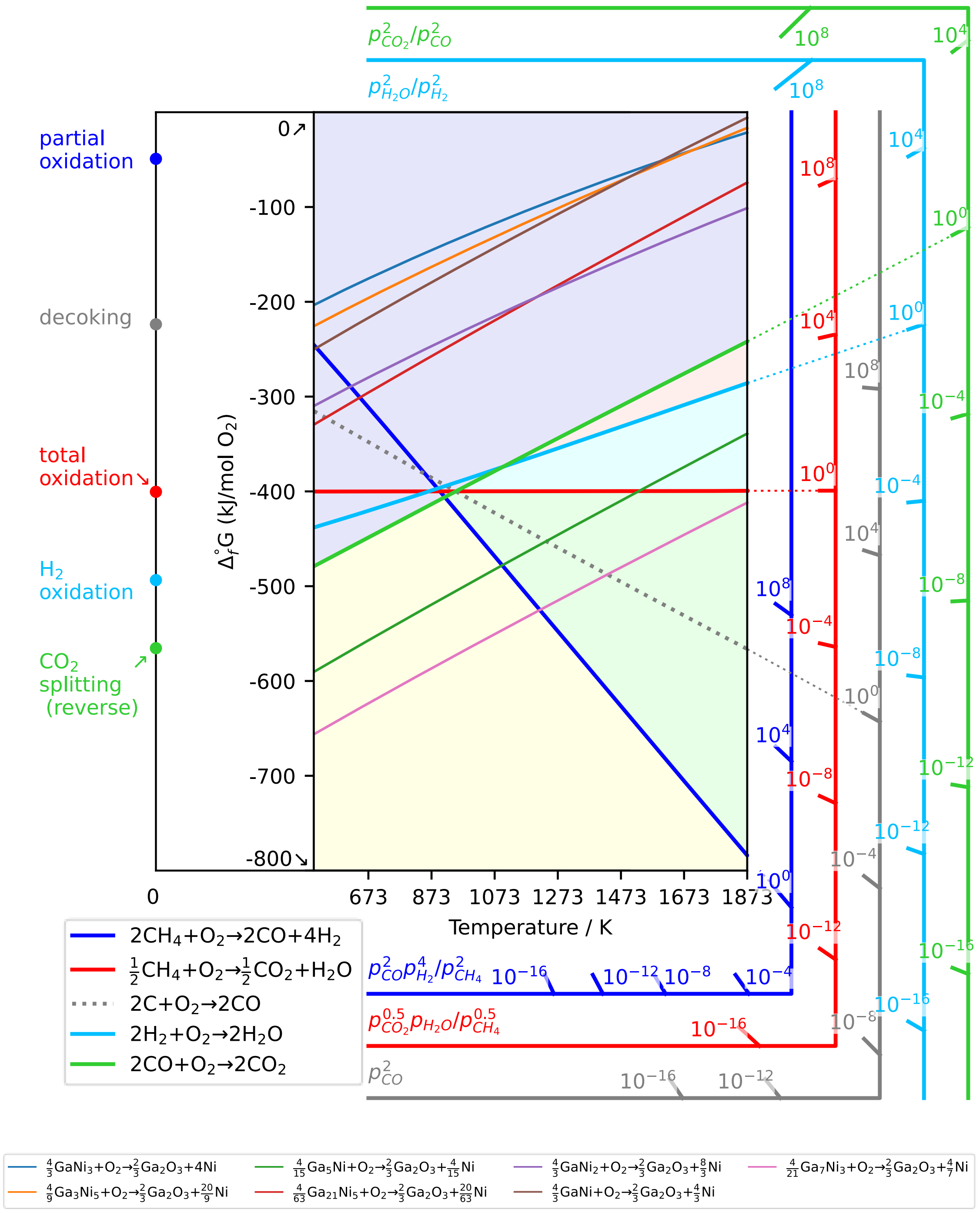

Fig. S23 Modified Ellingham diagram for Ga-Ni alloy oxygen carriers during chemical looping.

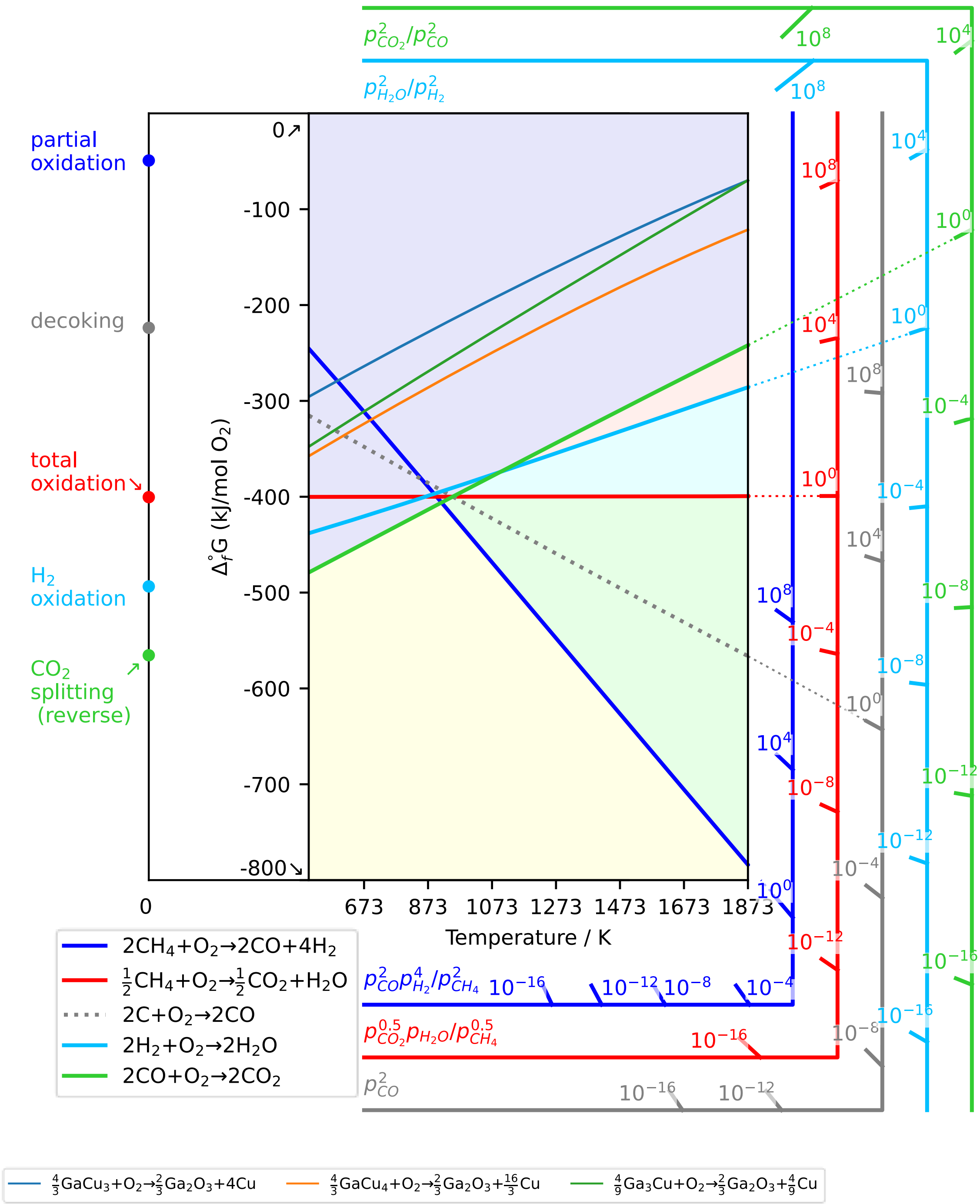

Fig. S24 Modified Ellingham diagram for Ga-Cu alloy oxygen carriers during chemical looping.

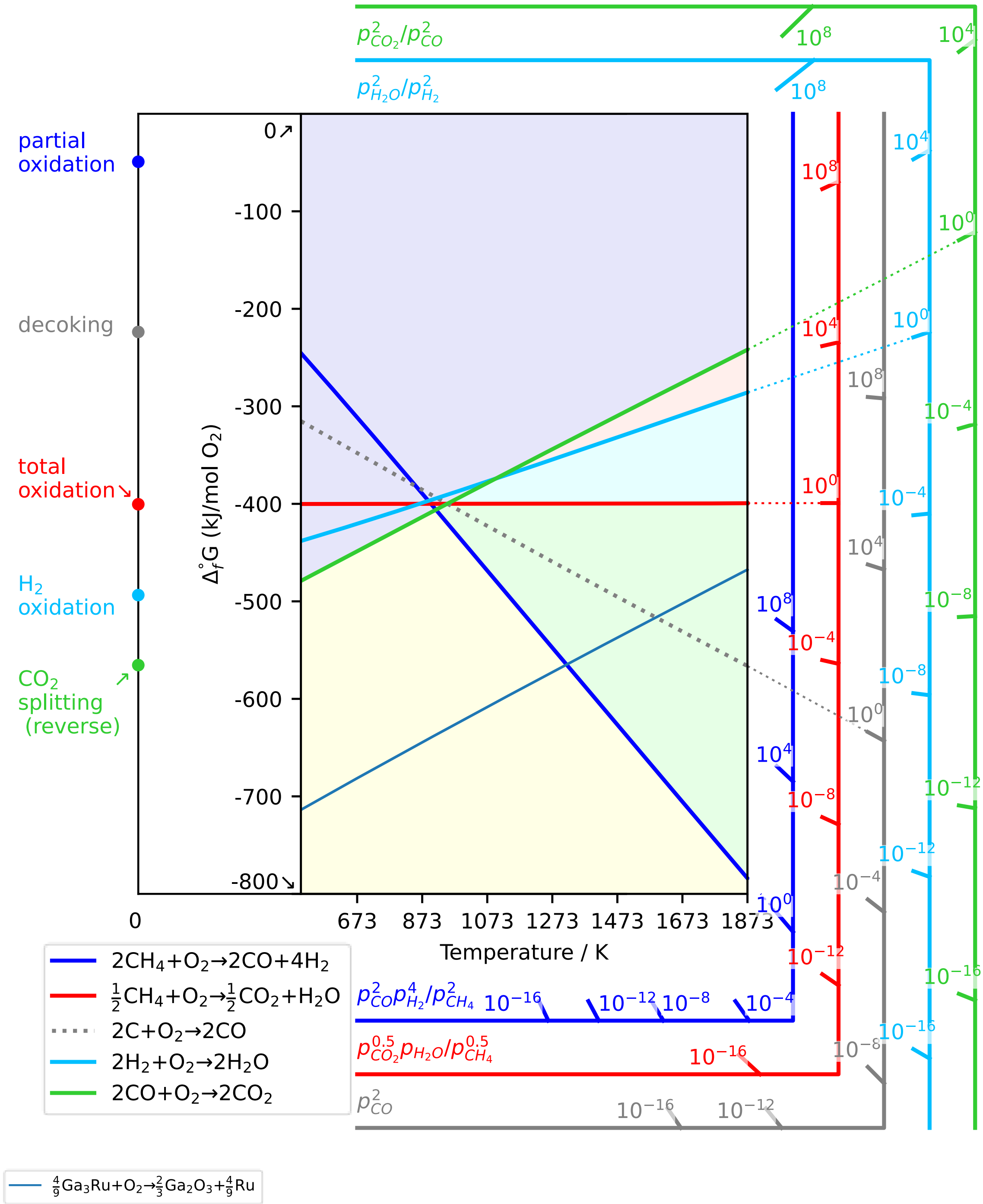

Fig. S25 Modified Ellingham diagram for Ga-Ru alloy oxygen carriers during chemical looping.

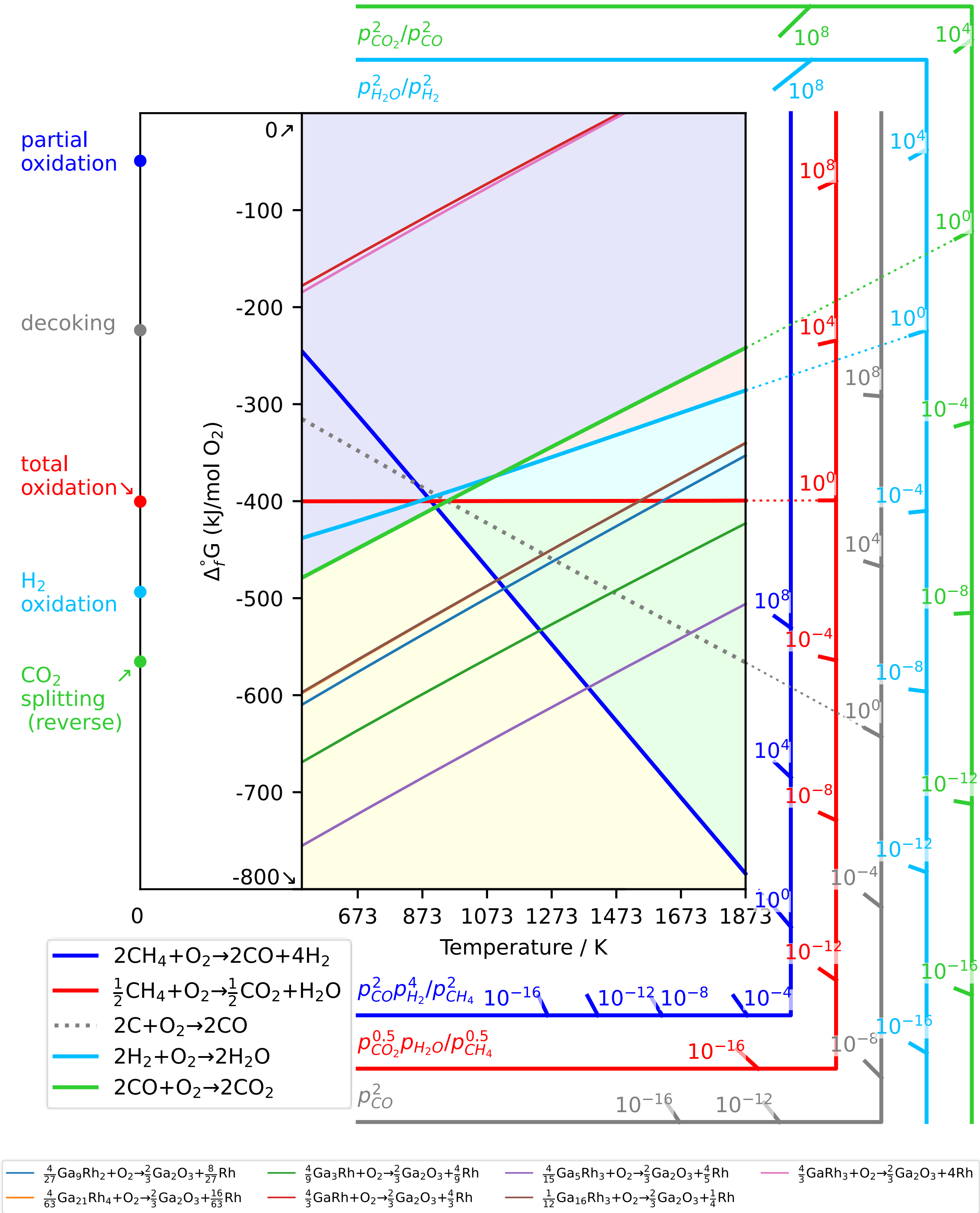

Fig. S26 Modified Ellingham diagram for Ga-Rh alloy oxygen carriers during chemical looping.

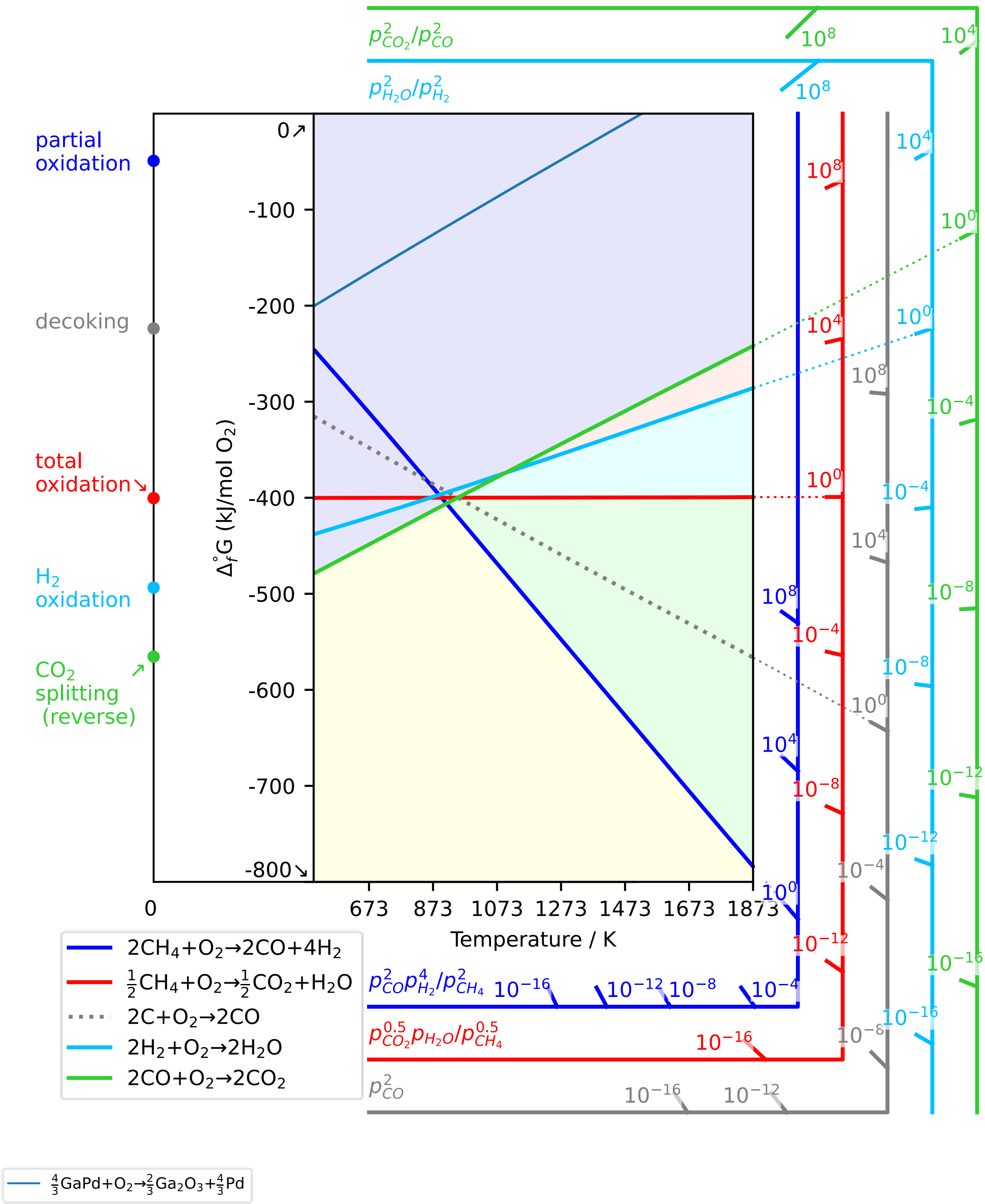

Fig. S27 Modified Ellingham diagram for Ga-Pd alloy oxygen carriers during chemical looping.

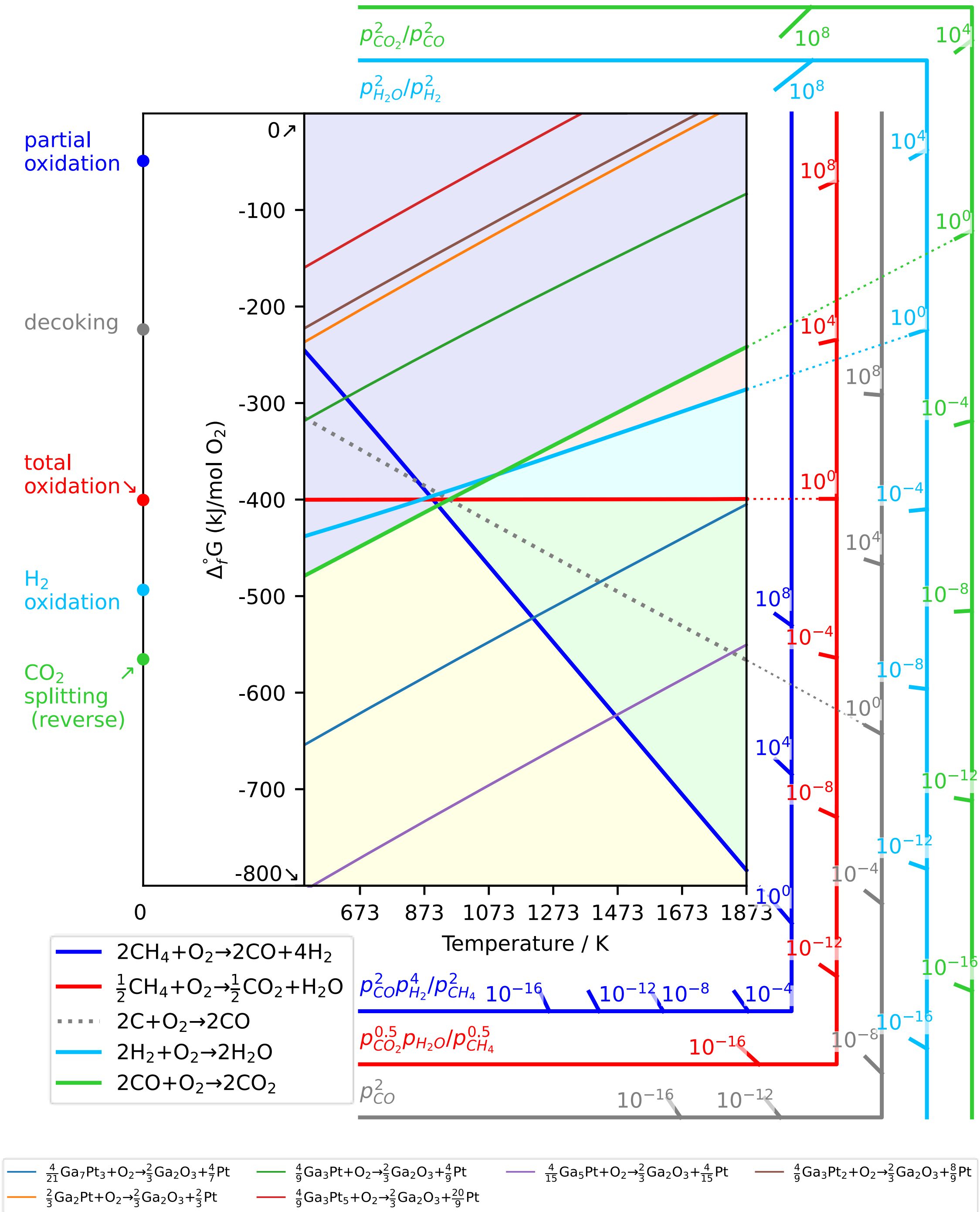

Fig. S28 Modified Ellingham diagram for Ga-Pt alloy oxygen carriers during chemical looping.

Table S1 Materials using NIST values

Material	Resource
V_2O_5	[1]
Fe	[1]
FeO	[1]
Fe_3O_4	[1]
Fe_2O_3	[1]
Co	[1]
CoO	[1]
Co_3O_4	[1]
Ni	[1]
Cu	[1]
Cu_2O	[1]
CuO	[1]

Table S2 Experimentally obtained formation enthalpies for fitting

Material	Formation enthalpy / kJ mol^{-1}	Resource
VO_2	-713.581	[9]
V_2O_5	-1550.59	[9]
MnO	-382.5	[10]
MnO_2	-522	[10]
FeO	-272.044	[9]
CoO	-237.735	[9]
Co_3O_4	-910.02	[9]
NiO	-239.7	[11]
Cu_2O	-170.707	[9]
CuO	-156.063	[9]
Ga_2O_3	-1089.1	[12]
SrO	-592.04	[1]
Y_2O_3	-1932.8	[13]
RuO_2	-312.3	[14]
Rh_2O_3	-405.53	[15]
PdO	-117.42	[16]
In_2O_3	-923.5	[17]
PtO_2	-80	[18]
La_2O_3	-1791.6	[19]
Ce_2O_3	-1799.8	[19]
CeO_2	-1090.4	[19]
Pr_2O_3	-1809.9	[19]
PrO_2	-959.1	[19]
WO_3	-842.91	[1]

Table S3 Gibbs energies of Fe-based alloy oxygen carriers at representative temperatures

	500 K	600 K	700 K	800 K	900 K	1000 K	1100 K	1200 K	1300 K	1400 K	1500 K	1600 K	1700 K	1800 K
4/9Fe3Ni+O2-> 2/3Fe2O3+4/9Ni	-458.35	-441.03	-424.26	-408.03	-392.33	-377.15	-362.37	-347.88	-333.63	-319.61	-305.82	-292.24	-278.86	-265.68
1/2Fe3Ni+O2-> 1/2Fe3O4+1/2Ni	-473.28	-457.06	-441.54	-426.75	-412.7	-399.2	-386.03	-373.15	-360.55	-348.19	-336.07	-324.17	-312.48	-300.98
2/3Fe3Ni+O2-> 2FeO+2/3Ni	-474.63	-462.22	-450.39	-439.07	-428.21	-417.77	-407.73	-398.07	-388.78	-379.83	-371.22	-362.93	-354.96	-347.3
4/3FeNi3+O2-> 2/3Fe2O3+4Ni	-431.38	-415.9	-401.45	-387.95	-375.28	-363.4	-352.2	-341.55	-331.41	-321.78	-312.65	-304	-295.83	-288.15
3/2FeNi3+O2-> 1/2Fe3O4+9/2Ni	-442.95	-428.8	-415.89	-404.16	-393.51	-383.73	-374.58	-366.03	-358.06	-350.63	-343.75	-337.4	-331.57	-326.25
2FeNi3+O2-> 2FeO+6Ni	-434.19	-424.54	-416.18	-408.96	-402.63	-397.15	-392.47	-388.58	-385.46	-383.08	-381.46	-380.57	-380.42	-381
2/3Fe2Ni+O2-> 2/3Fe2O3+2/3Ni	-467.08	-449.44	-432.39	-415.9	-399.95	-384.54	-369.55	-354.85	-340.42	-326.24	-312.3	-298.59	-285.1	-271.82
3/4Fe2Ni+O2-> 1/2Fe3O4+3/4Ni	-483.11	-466.54	-450.69	-435.6	-421.26	-407.51	-394.1	-381	-368.19	-355.65	-343.36	-331.31	-319.49	-307.88
1Fe2Ni+O2-> 2FeO+1Ni	-487.74	-474.85	-462.58	-450.87	-439.63	-428.85	-418.49	-408.53	-398.97	-389.77	-380.94	-372.46	-364.32	-356.51
4/3FeNi+O2-> 2/3Fe2O3+4/3Ni	-446.33	-429.51	-413.36	-397.87	-382.97	-368.66	-354.82	-341.32	-328.14	-315.27	-302.68	-290.38	-278.34	-266.57
3/2FeNi+O2->	-459.76	-444.11	-429.29	-415.31	-402.16	-389.64	-377.52	-365.78	-354.38	-343.31	-332.54	-322.07	-311.89	-301.98

1/2Fe3O4+3/2Ni														
2FeNi+O2-> 2FeO+2Ni	-456.6	-444.95	-434.05	-423.82	-414.16	-405.03	-396.39	-388.24	-380.55	-373.31	-366.51	-360.14	-354.19	-348.64
4/3FeNi2+O2-> 2/3Fe2O3+8/3Ni	-1728.57	-1720.65	-1714.33	-1709.46	-1705.85	-1703.44	-1702.05	-1701.52	-1701.78	-1702.8	-1704.52	-1706.93	-1710	-1713.71
3/2FeNi2+O2-> 1/2Fe3O4+3Ni	-1902.28	-1896.65	-1892.88	-1890.85	-1890.41	-1891.27	-1893.17	-1896	-1899.72	-1904.28	-1909.61	-1915.7	-1922.51	-1930.01
2FeNi2+O2-> 2FeO+4Ni	-2379.97	-2381.67	-2385.5	-2391.21	-2398.49	-2407.21	-2417.25	-2428.54	-2441.01	-2454.61	-2469.27	-2484.97	-2501.68	-2519.35
4/3FeCo3+O2-> 2/3Fe2O3+4Co	-451.02	-433.35	-416.57	-400.87	-386.05	-372.16	-359.13	-346.91	-335.52	-325.09	-315.51	-306.51	-298.03	-290.01
3/2FeCo3+O2-> 1/2Fe3O4+9/2Co	-465.03	-448.43	-432.9	-418.69	-405.63	-393.58	-382.38	-372.06	-362.68	-354.36	-346.97	-340.23	-334.03	-328.35
2FeCo3+O2-> 2FeO+6Co	-463.64	-450.71	-438.87	-428.33	-418.78	-410.28	-402.87	-396.62	-391.62	-388.05	-385.75	-384.34	-383.71	-383.8
4/9Fe3Co+O2-> 2/3Fe2O3+4/9Co	-453.65	-436.93	-420.76	-405.15	-390.07	-375.53	-361.41	-347.6	-334.08	-320.83	-307.85	-295.1	-282.54	-270.18
1/2Fe3Co+O2-> 1/2Fe3O4+1/2Co	-467.99	-452.46	-437.61	-423.51	-410.16	-397.38	-384.95	-372.84	-361.05	-349.57	-338.36	-327.38	-316.62	-306.04
2/3Fe3Co+O2-> 2FeO+2/3Co	-467.58	-456.09	-445.15	-434.75	-424.82	-415.34	-406.29	-397.66	-389.45	-381.66	-374.27	-367.22	-360.48	-354.06
4/39Fe13Co3+O2-> 2/3Fe2O3+4/13Co	-455.42	-438.55	-422.21	-406.41	-391.13	-376.37	-362.01	-347.95	-334.14	-320.6	-307.29	-294.19	-281.29	-268.57

3/26Fe13Co3+O2-> 1/2Fe3O4+9/26Co	-469.99	-454.28	-439.25	-424.93	-411.35	-398.32	-385.62	-373.23	-361.13	-349.3	-337.73	-326.37	-315.21	-304.23
2/13Fe13Co3+O2-> 2FeO+6/13Co	-470.24	-458.51	-447.33	-436.64	-426.41	-416.6	-407.19	-398.18	-389.55	-381.31	-373.43	-365.87	-358.61	-351.63
4/45Fe15Co+O2-> 2/3Fe2O3+4/45Co	-458.54	-441.45	-424.87	-408.79	-393.21	-378.12	-363.41	-348.96	-334.74	-320.73	-306.93	-293.31	-279.87	-266.59
1/10Fe15Co+O2-> 1/2Fe3O4+1/10Co	-473.5	-457.55	-442.23	-427.6	-413.68	-400.29	-387.19	-374.37	-361.79	-349.45	-337.32	-325.38	-313.61	-302
2/15Fe15Co+O2-> 2FeO+2/15Co	-474.92	-462.86	-451.31	-440.21	-429.52	-419.22	-409.28	-399.7	-390.44	-381.51	-372.88	-364.54	-356.47	-348.67
4/33Fe11Co5+O2-> 2/3Fe2O3+20/33Co	-451.28	-434.59	-418.46	-402.91	-387.91	-373.47	-359.47	-345.79	-332.43	-319.38	-306.63	-294.11	-281.8	-269.71
3/22Fe11Co5+O2-> 1/2Fe3O4+15/22Co	-465.33	-449.83	-435.02	-420.99	-407.73	-395.05	-382.76	-370.81	-359.2	-347.94	-336.98	-326.27	-315.78	-305.51
2/11Fe11Co5+O2-> 2FeO+10/11Co	-464.03	-452.57	-441.7	-431.39	-421.58	-412.25	-403.37	-394.95	-386.98	-379.49	-372.43	-365.73	-359.38	-353.35
4/27Fe9Co7+O2-> 2/3Fe2O3+28/27Co	-444.6	-427.81	-411.62	-396.08	-381.13	-366.77	-352.92	-339.45	-326.37	-313.68	-301.34	-289.29	-277.5	-265.94
1/6Fe9Co7+O2-> 1/2Fe3O4+7/6Co	-457.82	-442.2	-427.33	-413.3	-400.09	-387.52	-375.39	-363.68	-352.38	-341.51	-331.03	-320.85	-310.94	-301.27
2/9Fe9Co7+O2-> 2FeO+14/9Co	-454.01	-442.41	-431.44	-421.14	-411.4	-402.21	-393.55	-385.44	-377.89	-370.92	-364.5	-358.51	-352.92	-347.7
4/3FeCo9+O2->	-1222.16	-1212.01	-1204.17	-1199.13	-1196.26	-1195.64	-1197.27	-1201.16	-1207.47	-1216.54	-1228.04	-1241.2	-1255.81	-1271.74

2/3Fe2O3+12Co														
3/2FeCo9+O2-> 1/2Fe3O4+27/2Co	-1332.57	-1324.42	-1318.95	-1316.74	-1317.12	-1320	-1325.29	-1333.09	-1343.62	-1357.23	-1373.57	-1391.75	-1411.54	-1432.8
2FeCo9+O2-> 2FeO+18Co	-1620.35	-1618.7	-1620.27	-1625.72	-1634.1	-1645.51	-1660.08	-1677.99	-1699.54	-1725.21	-1754.54	-1786.38	-1820.39	-1856.39
4/3FeCo+O2-> 2/3Fe2O3+4/3Co	-453.68	-436.74	-420.43	-404.8	-389.8	-375.43	-361.59	-348.18	-335.2	-322.66	-310.54	-298.72	-287.19	-275.92
3/2FeCo+O2-> 1/2Fe3O4+3/2Co	-468.03	-452.25	-437.24	-423.12	-409.85	-397.26	-385.14	-373.49	-362.31	-351.63	-341.38	-331.46	-321.85	-312.5
2FeCo+O2-> 2FeO+2Co	-467.63	-455.8	-444.65	-434.23	-424.41	-415.18	-406.55	-398.53	-391.13	-384.41	-378.29	-372.66	-367.46	-362.67
4/21Fe7Co+O2-> 2/3Fe2O3+4/21Co	-456.8	-439.79	-423.3	-407.33	-391.87	-376.91	-362.35	-348.05	-334.01	-320.2	-306.61	-293.21	-280	-266.96
3/14Fe7Co+O2-> 1/2Fe3O4+3/14Co	-471.54	-455.68	-440.47	-425.96	-412.18	-398.93	-386	-373.35	-360.98	-348.85	-336.95	-325.26	-313.75	-302.41
2/7Fe7Co+O2-> 2FeO+2/7Co	-472.31	-460.38	-448.96	-438.02	-427.52	-417.41	-407.69	-398.34	-389.35	-380.71	-372.4	-364.39	-356.67	-349.22
4/3FeCu+O2-> 2/3Fe2O3+4/3Cu	-498.62	-481.68	-465.28	-449.43	-434.11	-419.33	-404.97	-390.91	-377.14	-363.65	-350.43	-337.5	-324.86	-312.53
3/2FeCu+O2-> 1/2Fe3O4+3/2Cu	-518.59	-502.8	-487.7	-473.32	-459.7	-446.65	-433.95	-421.57	-409.5	-397.73	-386.26	-375.08	-364.22	-353.69
2FeCu+O2-> 2FeO+2Cu	-535.04	-523.21	-511.93	-501.17	-490.88	-481.04	-471.62	-462.63	-454.05	-445.88	-438.13	-430.82	-423.96	-417.58

4/9Fe3Cu+O2-> 2/3Fe2O3+4/9Cu	-468.76	-451.24	-434.23	-417.73	-401.73	-386.24	-371.13	-356.29	-341.69	-327.31	-313.16	-299.21	-285.48	-271.96
1/2Fe3Cu+O2-> 1/2Fe3O4+1/2Cu	-485	-468.56	-452.76	-437.66	-423.27	-409.42	-395.88	-382.62	-369.61	-356.85	-344.32	-332.01	-319.92	-308.04
2/3Fe3Cu+O2-> 2FeO+2/3Cu	-490.26	-477.54	-465.35	-453.61	-442.31	-431.4	-420.86	-410.69	-400.87	-391.38	-382.22	-373.39	-364.89	-356.72
4/3FeCu3+O2-> 2/3Fe2O3+4Cu	-501.43	-484.83	-468.88	-453.57	-438.9	-424.86	-411.35	-398.27	-385.61	-373.38	-361.61	-350.34	-339.63	-329.52
3/2FeCu3+O2-> 1/2Fe3O4+9/2Cu	-521.75	-506.35	-491.75	-477.98	-465.08	-452.87	-441.13	-429.85	-419.03	-408.68	-398.83	-389.53	-380.83	-372.8
2FeCu3+O2-> 2FeO+6Cu	-539.25	-527.94	-517.33	-507.38	-498.06	-489.33	-481.2	-473.67	-466.75	-460.48	-454.9	-450.09	-446.11	-443.06
4/3FeCu4+O2-> 2/3Fe2O3+16/3Cu	-495.72	-479.13	-463.23	-448.02	-433.49	-419.66	-406.4	-393.63	-381.34	-369.56	-358.34	-347.72	-337.78	-328.6
3/2FeCu4+O2-> 1/2Fe3O4+6Cu	-515.32	-499.93	-485.39	-471.74	-459	-447.02	-435.56	-424.62	-414.22	-404.39	-395.15	-386.59	-378.76	-371.76
2FeCu4+O2-> 2FeO+8Cu	-530.69	-519.38	-508.85	-499.06	-489.95	-481.53	-473.77	-466.7	-460.35	-454.76	-449.99	-446.15	-443.34	-441.69
4/3FeRh+O2-> 2/3Fe2O3+4/3Rh	-448.96	-431.1	-413.84	-397.16	-381.04	-365.48	-350.35	-335.52	-320.95	-306.64	-292.56	-278.7	-265.04	-251.58
3/2FeRh+O2-> 1/2Fe3O4+3/2Rh	-462.72	-445.9	-429.83	-414.52	-400	-386.07	-372.5	-359.25	-346.29	-333.6	-321.15	-308.93	-296.92	-285.11
2FeRh+O2->	-460.55	-447.34	-434.77	-422.76	-411.28	-400.26	-389.69	-379.53	-369.77	-360.37	-351.32	-342.62	-334.23	-326.15

2FeO+2Rh														
4/9Fe3Rh+O2-> 2/3Fe2O3+4/9Rh	-455.96	-438.6	-421.74	-405.36	-389.47	-374.07	-359.04	-344.25	-329.68	-315.3	-301.12	-287.11	-273.27	-259.59
1/2Fe3Rh+O2-> 1/2Fe3O4+1/2Rh	-470.6	-454.34	-438.71	-423.74	-409.48	-395.73	-382.27	-369.07	-356.1	-343.35	-330.78	-318.4	-306.18	-294.12
2/3Fe3Rh+O2-> 2FeO+2/3Rh	-471.06	-458.59	-446.61	-435.07	-423.92	-413.15	-402.73	-392.63	-382.85	-373.37	-364.17	-355.24	-346.58	-338.16
4/3FeRh3+O2-> 2/3Fe2O3+4Rh	-2378.89	-2361.03	-2343.67	-2326.79	-2310.4	-2294.5	-2278.96	-2263.67	-2248.59	-2233.72	-2219.03	-2204.51	-2190.17	-2175.98
3/2FeRh3+O2-> 1/2Fe3O4+9/2Rh	-2633.89	-2617.07	-2600.88	-2585.35	-2570.53	-2556.21	-2542.19	-2528.42	-2514.88	-2501.56	-2488.43	-2475.48	-2462.69	-2450.06
2FeRh3+O2-> 2FeO+6Rh	-3355.45	-3342.23	-3329.51	-3317.21	-3305.32	-3293.79	-3282.61	-3271.76	-3261.23	-3250.98	-3241.03	-3231.34	-3221.92	-3212.75
4/3FeRu+O2-> 2/3Fe2O3+4/3Ru	101.73	118.95	135.68	151.91	167.66	182.93	197.82	212.48	226.91	241.15	255.2	269.08	282.79	296.34
3/2FeRu+O2-> 1/2Fe3O4+3/2Ru	156.8	172.91	188.38	203.19	217.3	230.89	244.2	257.24	270.06	282.67	295.08	307.31	319.38	331.29
2FeRu+O2-> 2FeO+2Ru	365.48	377.74	389.51	400.84	411.78	422.35	432.56	442.46	452.04	461.32	470.32	479.04	487.51	495.72
4/3FePd3+O2-> 2/3Fe2O3+4Pd	-406.76	-388.07	-369.87	-352.15	-334.93	-318.18	-301.81	-285.68	-269.76	-254.04	-238.51	-223.16	-207.97	-192.94
3/2FePd3+O2-> 1/2Fe3O4+9/2Pd	-415.25	-397.49	-380.36	-363.89	-348.12	-332.86	-317.89	-303.18	-288.69	-274.42	-260.35	-246.45	-232.72	-219.15

2FePd3+O2-> 2FeO+6Pd	-397.25	-382.79	-368.81	-355.26	-342.1	-329.32	-316.88	-304.77	-292.97	-281.47	-270.25	-259.31	-248.63	-238.2
4/9Fe3Pd+O2-> 2/3Fe2O3+4/9Pd	-466.29	-448.58	-431.36	-414.64	-398.41	-382.66	-367.28	-352.15	-337.23	-322.51	-307.98	-293.63	-279.45	-265.42
1/2Fe3Pd+O2-> 1/2Fe3O4+1/2Pd	-482.22	-465.56	-449.54	-434.19	-419.53	-405.39	-391.55	-377.96	-364.6	-351.45	-338.5	-325.74	-313.13	-300.69
2/3Fe3Pd+O2-> 2FeO+2/3Pd	-486.55	-473.56	-461.05	-448.99	-437.32	-426.03	-415.09	-404.48	-394.18	-384.18	-374.46	-365.02	-355.84	-346.92
2/3Fe2Pd+O2-> 2/3Fe2O3+2/3Pd	-474.76	-457.14	-440.09	-423.58	-407.61	-392.17	-377.13	-362.38	-347.87	-333.6	-319.54	-305.69	-292.03	-278.55
3/4Fe2Pd+O2-> 1/2Fe3O4+3/4Pd	-491.75	-475.2	-459.36	-444.24	-429.88	-416.09	-402.63	-389.47	-376.57	-363.93	-351.51	-339.3	-327.28	-315.45
1Fe2Pd+O2-> 2FeO+1Pd	-499.25	-486.4	-474.14	-462.4	-451.13	-440.29	-429.87	-419.83	-410.15	-400.81	-391.8	-383.11	-374.71	-366.6
4/9Fe3Pt+O2-> 2/3Fe2O3+4/9Pt	-444.81	-427.64	-410.97	-394.79	-379.1	-363.9	-349.06	-334.46	-320.08	-305.9	-291.91	-278.1	-264.45	-250.96
1/2Fe3Pt+O2-> 1/2Fe3O4+1/2Pt	-458.05	-442.01	-426.6	-411.86	-397.81	-384.28	-371.04	-358.06	-345.31	-332.77	-320.43	-308.26	-296.26	-284.42
2/3Fe3Pt+O2-> 2FeO+2/3Pt	-454.32	-442.15	-430.46	-419.21	-408.36	-397.89	-387.76	-377.95	-368.46	-359.27	-350.36	-341.72	-333.35	-325.22
2/3Fe2Pt+O2-> 2/3Fe2O3+2/3Pt	-457.57	-439.7	-422.35	-405.5	-389.16	-373.31	-357.83	-342.62	-327.62	-312.84	-298.25	-283.85	-269.62	-255.55
3/4Fe2Pt+O2->	-472.4	-455.58	-439.4	-423.9	-409.12	-394.87	-380.92	-367.24	-353.79	-340.58	-327.56	-314.73	-302.08	-289.58

1/2Fe3O4+3/4Pt														
1Fe2Pt+O2-> 2FeO+1Pt	-473.46	-460.24	-447.53	-435.28	-423.44	-412	-400.92	-390.18	-379.77	-369.67	-359.87	-350.35	-341.1	-332.11
4/3FePt+O2-> 2/3Fe2O3+4/3Pt	-399.77	-382.58	-365.89	-349.68	-333.96	-318.73	-303.86	-289.23	-274.82	-260.61	-246.59	-232.74	-219.06	-205.54
3/2FePt+O2-> 1/2Fe3O4+3/2Pt	-407.38	-391.32	-375.88	-361.1	-347.03	-333.47	-320.2	-307.18	-294.39	-281.82	-269.44	-257.23	-245.2	-233.32
2FePt+O2-> 2FeO+2Pt	-386.77	-374.56	-362.84	-351.55	-340.65	-330.13	-319.96	-310.11	-300.57	-291.33	-282.37	-273.69	-265.26	-257.09
4/3FePt3+O2-> 2/3Fe2O3+4Pt	-367.18	-350.85	-335.02	-319.68	-304.82	-290.45	-276.45	-262.69	-249.14	-235.8	-222.64	-209.65	-196.84	-184.18
3/2FePt3+O2-> 1/2Fe3O4+9/2Pt	-370.72	-355.62	-341.15	-327.35	-314.25	-301.66	-289.36	-277.31	-265.5	-253.9	-242.49	-231.26	-220.2	-209.29
2FePt3+O2-> 2FeO+6Pt	-337.88	-326.97	-316.54	-306.54	-296.95	-287.72	-278.84	-270.29	-262.05	-254.1	-246.44	-239.05	-231.93	-225.05

Table S4 Gibbs energies of Mn-based alloy oxygen carriers at representative temperatures

	500 K	600 K	700 K	800 K	900 K	1000 K	1100 K	1200 K	1300 K	1400 K	1500 K	1600 K	1700 K	1800 K
1MnNi3+O2-> 1MnO2+3Ni	-387.02	-369.66	-352.85	-336.55	-320.63	-305.08	-289.87	-275	-260.46	-246.23	-232.32	-218.72	-205.43	-192.45
2MnNi3+O2-> 2MnO+6Ni	-606.42	-594.27	-583.19	-573.02	-563.53	-554.67	-546.42	-538.74	-531.63	-525.08	-519.09	-513.64	-508.75	-504.41
4/3MnNi3+O2-> 2/3Mn2O3+4Ni	-495.91	-480.13	-465.05	-450.58	-436.57	-423	-409.83	-397.06	-384.67	-372.67	-361.04	-349.79	-338.91	-328.41
1MnNi+O2-> 1MnO2+1Ni	-408.73	-389.54	-370.63	-351.99	-333.57	-315.36	-297.34	-279.5	-261.84	-244.35	-227.02	-209.85	-192.83	-175.96
2MnNi+O2-> 2MnO+2Ni	-649.85	-634.03	-618.74	-603.9	-589.4	-575.23	-561.35	-547.74	-534.41	-521.32	-508.49	-495.9	-483.54	-471.42
4/3MnNi+O2-> 2/3Mn2O3+4/3Ni	-524.86	-506.63	-488.75	-471.17	-453.82	-436.7	-419.78	-403.06	-386.52	-370.16	-353.98	-337.96	-322.11	-306.42
1/3Mn3Co+O2-> 1MnO2+1/3Co	-967.51	-948.99	-930.66	-912.53	-894.57	-876.78	-859.15	-841.67	-824.34	-807.17	-790.14	-773.22	-756.4	-739.67
2/3Mn3Co+O2-> 2MnO+2/3Co	-1767.4	-1752.94	-1738.8	-1724.98	-1711.41	-1698.08	-1684.97	-1672.07	-1659.4	-1646.96	-1634.72	-1622.63	-1610.68	-1598.85
4/9Mn3Co+O2-> 2/3Mn2O3+4/9Co	-1269.9	-1252.57	-1235.46	-1218.56	-1201.83	-1185.27	-1168.86	-1152.61	-1136.52	-1120.58	-1104.79	-1089.11	-1073.53	-1058.04
1MnCo3+O2-> 1MnO2+3Co	-441.02	-423.2	-405.82	-389.04	-372.69	-356.81	-341.41	-326.53	-312.23	-298.58	-285.5	-272.81	-260.46	-248.4
2MnCo3+O2->	-714.43	-701.36	-689.13	-678	-667.65	-658.12	-649.48	-641.8	-635.17	-629.77	-625.45	-621.83	-618.8	-616.31

2MnO+6Co														
4/3MnCo3+O2-> 2/3Mn2O3+4Co	-567.92	-551.52	-535.68	-520.57	-505.99	-491.96	-478.54	-465.76	-453.7	-442.46	-431.95	-421.91	-412.27	-403
1MnCu3+O2-> 1MnO2+3Cu	-1411.81	-1392.79	-1374.03	-1355.54	-1337.29	-1319.3	-1301.54	-1284.02	-1266.76	-1249.76	-1233.06	-1216.67	-1200.65	-1185.04
2MnCu3+O2-> 2MnO+6Cu	-2656.01	-2640.53	-2625.54	-2610.99	-2596.85	-2583.11	-2569.75	-2556.78	-2544.23	-2532.14	-2520.55	-2509.54	-2499.18	-2489.58
4/3MnCu3+O2-> 2/3Mn2O3+4Cu	-1862.3	-1844.3	-1826.62	-1809.23	-1792.12	-1775.29	-1758.72	-1742.42	-1726.41	-1710.71	-1695.35	-1680.39	-1665.86	-1651.85
1/4Mn4Cu+O2-> 1MnO2+1/4Cu	-433.58	-414.77	-396.13	-377.65	-359.31	-341.11	-323.04	-305.09	-287.25	-269.51	-251.88	-234.34	-216.9	-199.56
1/2Mn4Cu+O2-> 2MnO+1/2Cu	-699.54	-684.51	-669.74	-655.22	-640.89	-626.74	-612.76	-598.92	-585.21	-571.64	-558.2	-544.88	-531.69	-518.63
1/3Mn4Cu+O2-> 2/3Mn2O3+1/3Cu	-557.99	-540.28	-522.75	-505.38	-488.15	-471.04	-454.06	-437.17	-420.39	-403.71	-387.12	-370.61	-354.2	-337.89
1/3Mn3Rh+O2-> 1MnO2+1/3Rh	-416.05	-396.95	-378.01	-359.22	-340.56	-322.04	-303.63	-285.32	-267.12	-249.01	-230.98	-213.03	-195.15	-177.35
2/3Mn3Rh+O2-> 2MnO+2/3Rh	-664.49	-648.87	-633.5	-618.36	-603.39	-588.59	-573.92	-559.38	-544.96	-530.63	-516.4	-502.26	-488.19	-474.2
4/9Mn3Rh+O2-> 2/3Mn2O3+4/9Rh	-534.62	-516.53	-498.59	-480.81	-463.15	-445.61	-428.17	-410.82	-393.56	-376.37	-359.25	-342.2	-325.2	-308.27
1MnRh+O2-> 1MnO2+1Rh	-384.36	-365.33	-346.46	-327.74	-309.16	-290.7	-272.36	-254.12	-235.98	-217.94	-199.98	-182.09	-164.28	-146.54

2MnRh+O2-> 2MnO+2Rh	-601.11	-585.63	-570.41	-555.4	-540.58	-525.91	-511.38	-496.98	-482.69	-468.5	-454.4	-440.38	-426.45	-412.58
4/3MnRh+O2-> 2/3Mn2O3+4/3Rh	-492.37	-474.37	-456.53	-438.84	-421.27	-403.82	-386.47	-369.21	-352.04	-334.94	-317.91	-300.95	-284.04	-267.19
1MnRu3+O2-> 1MnO2+3Ru	-859.53	-841.52	-823.68	-805.98	-788.42	-771	-753.68	-736.48	-719.38	-702.36	-685.43	-668.58	-651.81	-635.1
2MnRu3+O2-> 2MnO+6Ru	-1551.45	-1538.01	-1524.83	-1511.88	-1499.11	-1486.5	-1474.04	-1461.7	-1449.47	-1437.34	-1425.31	-1413.37	-1401.5	-1389.7
4/3MnRu3+O2-> 2/3Mn2O3+4Ru	-1125.93	-1109.29	-1092.81	-1076.49	-1060.3	-1044.22	-1028.24	-1012.36	-996.56	-980.84	-965.19	-949.6	-934.07	-918.6
1MnRu+O2-> 1MnO2+1Ru	19.65	39.16	58.51	77.71	96.78	115.71	134.53	153.24	171.85	190.37	208.8	227.16	245.44	263.65
2MnRu+O2-> 2MnO+2Ru	206.92	223.35	239.54	255.5	271.29	286.91	302.39	317.74	332.98	348.12	363.16	378.11	392.99	407.79
4/3MnRu+O2-> 2/3Mn2O3+4/3Ru	46.31	64.96	83.43	101.77	119.97	138.06	156.04	173.93	191.74	209.47	227.12	244.72	262.25	279.72
1MnPd3+O2-> 1MnO2+3Pd	-389.94	-370.64	-351.5	-332.5	-313.64	-294.91	-276.3	-257.79	-239.38	-221.07	-202.84	-184.69	-166.61	-148.6
2MnPd3+O2-> 2MnO+6Pd	-612.27	-596.24	-580.47	-564.92	-549.54	-534.33	-519.26	-504.32	-489.49	-474.76	-460.12	-445.57	-431.1	-416.71
4/3MnPd3+O2-> 2/3Mn2O3+4Pd	-499.81	-481.44	-463.24	-445.18	-427.25	-409.44	-391.73	-374.11	-356.57	-339.12	-321.73	-304.41	-287.14	-269.94
1/7Mn7Pd9+O2->	-369.74	-350.09	-330.59	-311.24	-292.02	-272.94	-253.97	-235.1	-216.33	-197.66	-179.07	-160.56	-142.12	-123.74

1MnO2+9/7Pd														
2/7Mn7Pd9+O2-> 2MnO+18/7Pd	-571.86	-555.14	-538.66	-522.4	-506.31	-490.39	-474.6	-458.94	-443.39	-427.94	-412.58	-397.31	-382.11	-366.99
4/21Mn7Pd9+O2-> 2/3Mn2O3+12/7Pd	-472.87	-454.04	-435.36	-416.83	-398.43	-380.14	-361.95	-343.86	-325.84	-307.9	-290.04	-272.23	-254.49	-236.8
1MnPd2+O2-> 1MnO2+2Pd	-1803.27	-1783.5	-1763.89	-1744.43	-1725.11	-1705.91	-1686.84	-1667.87	-1648.99	-1630.22	-1611.52	-1592.91	-1574.36	-1555.89
2MnPd2+O2-> 2MnO+4Pd	-3438.92	-3421.97	-3405.27	-3388.78	-3372.48	-3356.34	-3340.34	-3324.47	-3308.71	-3293.05	-3277.49	-3262.01	-3246.61	-3231.29
4/3MnPd2+O2-> 2/3Mn2O3+8/3Pd	-2384.24	-2365.26	-2346.44	-2327.76	-2309.21	-2290.78	-2272.45	-2254.21	-2236.05	-2217.98	-2199.97	-2182.03	-2164.15	-2146.33
1/3Mn3Pd5+O2-> 1MnO2+5/3Pd	-358.38	-338.78	-319.33	-300.02	-280.85	-261.8	-242.87	-224.04	-205.31	-186.67	-168.12	-149.64	-131.23	-112.89
2/3Mn3Pd5+O2-> 2MnO+10/3Pd	-549.16	-532.52	-516.14	-499.96	-483.96	-468.11	-452.4	-436.82	-421.34	-405.96	-390.68	-375.47	-360.35	-345.29
4/9Mn3Pd5+O2-> 2/3Mn2O3+20/9Pd	-457.73	-438.96	-420.35	-401.87	-383.53	-365.29	-347.15	-329.11	-311.14	-293.25	-275.43	-257.67	-239.97	-222.33
1MnPd+O2-> 1MnO2+1Pd	-380.85	-361.21	-341.73	-322.4	-303.2	-284.13	-265.18	-246.33	-227.59	-208.93	-190.36	-171.87	-153.45	-135.1
2MnPd+O2-> 2MnO+2Pd	-594.08	-577.39	-560.94	-544.71	-528.66	-512.78	-497.03	-481.4	-465.89	-450.48	-435.17	-419.94	-404.79	-389.71
4/3MnPd+O2-> 2/3Mn2O3+4/3Pd	-487.68	-468.87	-450.22	-431.71	-413.33	-395.07	-376.9	-358.83	-340.85	-322.94	-305.1	-287.32	-269.6	-251.94

1/11Mn11Pd21+O2-> 1MnO2+21/11Pd	-358.23	-338.64	-319.19	-299.9	-280.74	-261.7	-242.78	-223.97	-205.26	-186.63	-168.09	-149.63	-131.24	-112.92
2/11Mn11Pd21+O2-> 2MnO+42/11Pd	-548.85	-532.24	-515.87	-499.71	-483.74	-467.92	-452.24	-436.68	-421.23	-405.89	-390.63	-375.46	-360.37	-345.35
4/33Mn11Pd21+O2-> 2/3Mn2O3+28/11Pd	-457.53	-438.77	-420.17	-401.71	-383.38	-365.16	-347.04	-329.02	-311.07	-293.2	-275.4	-257.67	-239.99	-222.37
1MnPt+O2-> 1MnO2+1Pt	-357.11	-338.09	-319.23	-300.52	-281.94	-263.5	-245.16	-226.94	-208.82	-190.78	-172.83	-154.96	-137.16	-119.44
2MnPt+O2-> 2MnO+2Pt	-546.6	-531.14	-515.94	-500.95	-486.15	-471.5	-457	-442.62	-428.35	-414.18	-400.11	-386.12	-372.21	-358.38
4/3MnPt+O2-> 2/3Mn2O3+4/3Pt	-456.03	-438.04	-420.22	-402.54	-384.99	-367.55	-350.22	-332.98	-315.82	-298.74	-281.72	-264.77	-247.89	-231.05
1/3Mn3Pt+O2-> 1MnO2+1/3Pt	-408.81	-390.17	-371.73	-353.45	-335.34	-317.38	-299.55	-281.85	-264.27	-246.79	-229.41	-212.12	-194.92	-177.79
2/3Mn3Pt+O2-> 2MnO+2/3Pt	-650.01	-635.31	-620.93	-606.82	-592.95	-579.27	-565.78	-552.44	-539.26	-526.2	-513.26	-500.44	-487.72	-475.09
4/9Mn3Pt+O2-> 2/3Mn2O3+4/9Pt	-524.97	-507.49	-490.21	-473.12	-456.19	-439.4	-422.74	-406.19	-389.75	-373.41	-357.16	-340.98	-324.89	-308.86
1MnPt3+O2-> 1MnO2+3Pt	-301.59	-283.77	-266.11	-248.59	-231.21	-213.95	-196.81	-179.78	-162.84	-145.99	-129.23	-112.54	-95.92	-79.37
2MnPt3+O2-> 2MnO+6Pt	-435.57	-422.51	-409.7	-397.1	-384.68	-372.42	-360.3	-348.29	-336.4	-324.6	-312.9	-301.27	-289.73	-278.25
4/3MnPt3+O2->	-382.01	-365.62	-349.39	-333.3	-317.34	-301.5	-285.75	-270.09	-254.52	-239.01	-223.58	-208.21	-192.9	-177.64

$2/3Mn_2O_3+4Pt$

Table S5 Gibbs energies of In-based alloy oxygen carriers at representative temperatures

	500 K	600 K	700 K	800 K	900 K	1000 K	1100 K	1200 K	1300 K	1400 K	1500 K	1600 K	1700 K	1800 K
4/21In7Ni3+O2-> 2/3In2O3+4/7Ni	-821.5	-802.94	-784.67	-766.67	-748.88	-731.3	-713.89	-696.64	-679.55	-662.6	-645.79	-629.1	-612.54	-596.1
4/3InNi+O2-> 2/3In2O3+4/3Ni	-494.38	-475.69	-457.41	-439.49	-421.84	-404.45	-387.3	-370.37	-353.65	-337.14	-320.81	-304.68	-288.73	-272.96
4/3InNi3+O2-> 2/3In2O3+4Ni	-498.07	-481.55	-465.79	-450.69	-436.09	-421.95	-408.26	-394.99	-382.13	-369.67	-357.61	-345.95	-334.67	-323.79
4/9In3Ni+O2-> 2/3In2O3+4/9Ni	-558.86	-542.86	-527.4	-512.4	-497.61	-483.12	-468.94	-455.06	-441.44	-428.06	-414.92	-402	-389.28	-376.75
4/27In9Ni13+O2-> 2/3In2O3+52/27Ni	-482.04	-464.06	-446.58	-429.51	-412.77	-396.34	-380.18	-364.29	-348.66	-333.28	-318.13	-303.22	-288.53	-274.08
4/9In3Ni2+O2-> 2/3In2O3+8/9Ni	-484.7	-466.72	-449.08	-431.74	-414.65	-397.78	-381.11	-364.63	-348.33	-332.19	-316.22	-300.39	-284.72	-269.19
4/3InNi2+O2-> 2/3In2O3+8/3Ni	-1383.17	-1365.39	-1348.2	-1331.53	-1315.25	-1299.34	-1283.78	-1268.54	-1253.61	-1238.99	-1224.68	-1210.65	-1196.92	-1183.48
4/9In3Co+O2-> 2/3In2O3+4/9Co	-838.15	-819.71	-801.53	-783.62	-765.92	-748.42	-731.12	-713.99	-697.05	-680.29	-663.69	-647.22	-630.87	-614.62
2/3In2Co+O2-> 2/3In2O3+2/3Co	-1105.71	-1087.39	-1069.37	-1051.65	-1034.17	-1016.92	-999.89	-983.08	-966.49	-950.12	-933.96	-917.95	-902.08	-886.34
4/9In3Cu+O2-> 2/3In2O3+4/9Cu	-542.31	-522.95	-503.97	-485.31	-466.93	-448.81	-430.92	-413.24	-395.76	-378.46	-361.34	-344.39	-327.61	-311
4/3InCu+O2->	-924.92	-905.63	-886.62	-867.85	-849.3	-830.96	-812.8	-794.82	-777.02	-759.4	-741.96	-724.71	-707.67	-690.85

2/3In2O3+4/3Cu														
4/3InCu2+O2-> 2/3In2O3+8/3Cu	-1183.21	-1165.72	-1148.74	-1132.22	-1116.13	-1100.42	-1085.08	-1070.08	-1055.42	-1041.12	-1027.17	-1013.6	-1000.44	-987.73
2/3In2Cu+O2-> 2/3In2O3+2/3Cu	-812.66	-793.75	-775.17	-756.88	-738.85	-721.05	-703.46	-686.06	-668.86	-651.82	-634.97	-618.28	-601.76	-585.42
1/3In4Cu9+O2-> 2/3In2O3+3Cu	-1573.73	-1553.79	-1534.2	-1514.93	-1495.95	-1477.24	-1458.8	-1440.62	-1422.71	-1405.07	-1387.74	-1370.75	-1354.12	-1337.91
4/21In7Cu10+O2-> 2/3In2O3+40/21Cu	-1023.21	-1003.94	-984.96	-966.25	-947.79	-929.54	-911.51	-893.69	-876.07	-858.66	-841.48	-824.53	-807.84	-791.45
4/27In9Cu11+O2-> 2/3In2O3+44/27Cu	-516.48	-497.2	-478.21	-459.47	-440.96	-422.67	-404.58	-386.68	-368.98	-351.47	-334.16	-317.07	-300.21	-283.61
4/9In3Rh+O2-> 2/3In2O3+4/9Rh	-985.73	-966.84	-948.18	-929.71	-911.42	-893.28	-875.28	-857.39	-839.62	-821.94	-804.36	-786.86	-769.44	-752.09
4/3InRh3+O2-> 2/3In2O3+4Rh	-2041.97	-2021.8	-2001.85	-1982.1	-1962.51	-1943.08	-1923.78	-1904.6	-1885.53	-1866.56	-1847.68	-1828.88	-1810.17	-1791.52
4/3InRh+O2-> 2/3In2O3+4/3Rh	-417.47	-399.26	-381.29	-363.51	-345.9	-328.44	-311.12	-293.92	-276.83	-259.84	-242.94	-226.12	-209.38	-192.71
4/9In3Ru+O2-> 2/3In2O3+4/9Ru	-860.97	-842.68	-824.61	-806.74	-789.05	-771.5	-754.1	-736.81	-719.63	-702.55	-685.56	-668.66	-651.83	-635.08
4/9In3Pd2+O2-> 2/3In2O3+8/9Pd	-417.83	-399.05	-380.49	-362.13	-343.95	-325.92	-308.02	-290.24	-272.57	-255	-237.53	-220.13	-202.82	-185.58
4/3InPd3+O2-> 2/3In2O3+4Pd	-287.4	-268.1	-249.03	-230.15	-211.45	-192.9	-174.48	-156.19	-138.01	-119.92	-101.94	-84.03	-66.21	-48.45

4/3InPd2+O2-> 2/3In2O3+8/3Pd	-1719.84	-1700.71	-1681.8	-1663.1	-1644.57	-1626.19	-1607.94	-1589.82	-1571.81	-1553.89	-1536.07	-1518.34	-1500.68	-1483.1
4/9In3Pd5+O2-> 2/3In2O3+20/9Pd	-1151.08	-1131.84	-1112.83	-1094.01	-1075.37	-1056.88	-1038.53	-1020.29	-1002.17	-984.14	-966.21	-948.36	-930.59	-912.9
4/3InPd+O2-> 2/3In2O3+4/3Pd	-390.86	-371.54	-352.46	-333.58	-314.87	-296.31	-277.89	-259.6	-241.41	-223.32	-205.32	-187.41	-169.58	-151.83
4/9In3Pd+O2-> 2/3In2O3+4/9Pd	-779.19	-759.74	-740.55	-721.57	-702.78	-684.16	-665.68	-647.33	-629.11	-610.99	-592.97	-575.05	-557.21	-539.45
4/21In7Pd3+O2-> 2/3In2O3+4/7Pd	-791.66	-772.83	-754.22	-735.81	-717.58	-699.49	-681.54	-663.71	-645.99	-628.36	-610.83	-593.39	-576.02	-558.72
4/9In3Pt2+O2-> 2/3In2O3+8/9Pt	-419.24	-401.07	-383.13	-365.39	-347.82	-330.41	-313.13	-295.97	-278.92	-261.97	-245.11	-228.34	-211.64	-195.02
4/3InPt3+O2-> 2/3In2O3+4Pt	-329.52	-312.39	-295.5	-278.8	-262.27	-245.89	-229.65	-213.53	-197.51	-181.6	-165.77	-150.03	-134.36	-118.77
4/27In9Pt13+O2-> 2/3In2O3+52/27Pt	-384.57	-366.28	-348.23	-330.41	-312.77	-295.29	-277.97	-260.77	-243.7	-226.73	-209.87	-193.09	-176.4	-159.8
4/3InPt+O2-> 2/3In2O3+4/3Pt	-454.23	-437.21	-420.56	-404.22	-388.16	-372.33	-356.73	-341.32	-326.09	-311.02	-296.1	-281.32	-266.67	-252.14
4/9In3Pt+O2-> 2/3In2O3+4/9Pt	-522.59	-507.7	-493.31	-479.37	-465.82	-452.61	-439.7	-427.07	-414.69	-402.55	-390.62	-378.88	-367.33	-355.95
4/9In3Pt5+O2-> 2/3In2O3+20/9Pt	-424.4	-406.36	-388.54	-370.93	-353.49	-336.2	-319.05	-302.02	-285.1	-268.28	-251.55	-234.91	-218.34	-201.85
4/15In5Pt11+O2->	-360.75	-343.16	-325.81	-308.66	-291.67	-274.84	-258.15	-241.57	-225.11	-208.74	-192.46	-176.27	-160.16	-144.12

2/3In2O3+44/15Pt														
2/3In2Pt+O2-> 2/3In2O3+2/3Pt	-428.54	-410.16	-392.01	-374.06	-356.28	-338.65	-321.16	-303.79	-286.54	-269.38	-252.31	-235.33	-218.43	-201.6
2/3In2Pt3+O2-> 2/3In2O3+2Pt	-1613.13	-1595.34	-1577.77	-1560.41	-1543.21	-1526.17	-1509.26	-1492.47	-1475.79	-1459.21	-1442.72	-1426.31	-1409.98	-1393.72
4/3InPt2+O2-> 2/3In2O3+8/3Pt	-2161.3	-2143.45	-2125.82	-2108.4	-2091.14	-2074.04	-2057.08	-2040.23	-2023.49	-2006.86	-1990.31	-1973.85	-1957.47	-1941.15
4/21In7Pt3+O2-> 2/3In2O3+4/7Pt	-813.48	-795	-776.75	-758.69	-740.81	-723.08	-705.48	-688.01	-670.64	-653.38	-636.2	-619.11	-602.1	-585.16
4/9In3Pt4+O2-> 2/3In2O3+16/9Pt	-1390.36	-1371.86	-1353.59	-1335.52	-1317.62	-1299.88	-1282.26	-1264.77	-1247.39	-1230.11	-1212.92	-1195.81	-1178.78	-1161.83

Table S6 Gibbs energies of Ga-based alloy oxygen carriers at representative temperatures

	500 K	600 K	700 K	800 K	900 K	1000 K	1100 K	1200 K	1300 K	1400 K	1500 K	1600 K	1700 K	1800 K
4/3GaNi3+O2-> 2/3Ga2O3+4Ni	-203.49	-187.02	-171.29	-156.19	-141.59	-127.45	-113.74	-100.45	-87.57	-75.09	-63	-51.31	-40.01	-29.11
4/9Ga3Ni5+O2-> 2/3Ga2O3+20/9Ni	-225.77	-208.37	-191.45	-174.98	-158.84	-143.03	-127.51	-112.27	-97.31	-82.62	-68.18	-54	-40.07	-26.39
1/3Ga4Ni3+O2-> 2/3Ga2O3+1Ni	-1128.75	-1110.4	-1092.38	-1074.66	-1057.18	-1039.92	-1022.86	-1006	-989.32	-972.81	-956.46	-940.28	-924.25	-908.37
4/15Ga5Ni+O2-> 2/3Ga2O3+4/15Ni	-590.45	-571.1	-551.99	-533.09	-514.37	-495.81	-477.39	-459.12	-440.96	-422.93	-405	-387.18	-369.45	-351.82
4/63Ga21Ni5+O2-> 2/3Ga2O3+20/63Ni	-329.65	-309.95	-290.5	-271.27	-252.23	-233.36	-214.65	-196.08	-177.65	-159.34	-141.15	-123.06	-105.09	-87.21
4/3GaNi2+O2-> 2/3Ga2O3+8/3Ni	-309.95	-292.32	-275.24	-258.65	-242.44	-226.57	-211.04	-195.83	-180.93	-166.32	-152.01	-137.98	-124.25	-110.79
4/3GaNi+O2-> 2/3Ga2O3+4/3Ni	-250.29	-230.82	-211.73	-192.97	-174.48	-156.23	-138.22	-120.43	-102.84	-85.45	-68.25	-51.24	-34.41	-17.76
4/21Ga7Ni3+O2-> 2/3Ga2O3+4/7Ni	-656.28	-637.27	-618.53	-600.04	-581.76	-563.66	-545.73	-527.96	-510.34	-492.85	-475.5	-458.28	-441.18	-424.19
4/9Ga3Co+O2-> 2/3Ga2O3+4/9Co	-842.64	-823.5	-804.6	-785.94	-767.48	-749.22	-731.14	-713.24	-695.51	-677.96	-660.57	-643.32	-626.17	-609.13
4/3GaCo+O2-> 2/3Ga2O3+4/3Co	-282.9	-265.33	-248.1	-231.25	-214.68	-198.42	-182.44	-166.77	-151.41	-136.4	-121.69	-107.21	-92.92	-78.8
4/3GaCo3+O2->	-297.94	-280.68	-264.02	-248.11	-232.77	-218.02	-203.89	-190.43	-177.71	-165.83	-154.7	-144.07	-133.85	-124.02

2/3Ga2O3+4Co														
4/3GaCu2+O2-> 2/3Ga2O3+8/3Cu	-1024.46	-1007.2	-990.47	-974.21	-958.4	-942.99	-927.95	-913.29	-898.98	-885.04	-871.47	-858.3	-845.55	-833.25
4/3GaCu3+O2-> 2/3Ga2O3+4Cu	-295.68	-277.13	-258.93	-241.05	-223.48	-206.21	-189.22	-172.53	-156.15	-140.1	-124.41	-109.12	-94.3	-80
1/3Ga4Cu9+O2-> 2/3Ga2O3+3Cu	-1428.15	-1408.5	-1389.16	-1370.11	-1351.32	-1332.8	-1314.52	-1296.49	-1278.72	-1261.22	-1244.01	-1227.13	-1210.61	-1194.51
4/3GaCu4+O2-> 2/3Ga2O3+16/3Cu	-357.62	-337.91	-318.58	-299.63	-281.03	-262.78	-244.88	-227.32	-210.14	-193.37	-177.05	-161.25	-146.03	-131.49
4/9Ga3Cu+O2-> 2/3Ga2O3+4/9Cu	-347.75	-326.44	-305.35	-284.47	-263.77	-243.24	-222.87	-202.63	-182.53	-162.56	-142.72	-123	-103.4	-83.93
4/27Ga9Rh2+O2-> 2/3Ga2O3+8/27Rh	-609.88	-590.29	-570.9	-551.69	-532.64	-513.73	-494.95	-476.28	-457.72	-439.25	-420.87	-402.58	-384.36	-366.21
4/63Ga21Rh4+O2-> 2/3Ga2O3+16/63Rh	-597.87	-578.19	-558.71	-539.41	-520.26	-501.26	-482.39	-463.63	-444.98	-426.43	-407.96	-389.58	-371.27	-353.03
4/9Ga3Rh+O2-> 2/3Ga2O3+4/9Rh	-669.1	-649.95	-631.08	-612.45	-594.04	-575.82	-557.78	-539.91	-522.17	-504.57	-487.1	-469.74	-452.48	-435.33
4/51Ga17Rh10+O2-> 2/3Ga2O3+40/51Rh	-1011.44	-992.3	-973.36	-954.6	-936	-917.54	-899.2	-880.98	-862.87	-844.85	-826.92	-809.07	-791.3	-773.6
4/3GaRh+O2-> 2/3Ga2O3+4/3Rh	-178	-159.24	-140.67	-122.28	-104.05	-85.97	-68.01	-50.16	-32.42	-14.78	2.77	20.24	37.64	54.96
4/15Ga5Rh3+O2-> 2/3Ga2O3+4/5Rh	-755.24	-736.21	-717.38	-698.72	-680.23	-661.87	-643.64	-625.53	-607.52	-589.61	-571.79	-554.04	-536.38	-518.78

1/12Ga16Rh3+O2-> 2/3Ga2O3+1/4Rh	-597.13	-577.52	-558.11	-538.88	-519.82	-500.9	-482.11	-463.45	-444.89	-426.43	-408.06	-389.78	-371.58	-353.45
4/3GaRh3+O2-> 2/3Ga2O3+4Rh	-184.7	-165.54	-146.57	-127.77	-109.13	-90.63	-72.26	-54	-35.84	-17.78	0.19	18.08	35.9	53.65
4/9Ga3Ru+O2-> 2/3Ga2O3+4/9Ru	-713.81	-694.99	-676.36	-657.92	-639.64	-621.49	-603.48	-585.58	-567.78	-550.08	-532.47	-514.94	-497.49	-480.11
4/3GaRu+O2-> 2/3Ga2O3+4/3Ru	318.51	337.84	356.98	375.94	394.74	413.4	431.93	450.35	468.65	486.87	504.99	523.03	540.99	558.89
4/15Ga5Pd13+O2-> 2/3Ga2O3+52/15Pd	-97.59	-77.97	-58.55	-39.31	-20.23	-1.29	17.53	36.23	54.82	73.32	91.72	110.05	128.3	146.48
4/9Ga3Pd7+O2-> 2/3Ga2O3+28/9Pd	-99.85	-80.23	-60.8	-41.55	-22.46	-3.51	15.31	34.01	52.61	71.11	89.53	107.86	126.11	144.29
4/3GaPd3+O2-> 2/3Ga2O3+4Pd	-119.03	-98.4	-78.01	-57.84	-37.86	-18.05	1.61	21.13	40.51	59.79	78.95	98.02	116.99	135.88
4/3GaPd+O2-> 2/3Ga2O3+4/3Pd	-200.55	-180.29	-160.23	-140.34	-120.61	-101.02	-81.56	-62.21	-42.97	-23.83	-4.78	14.19	33.08	51.9
4/3GaPd2+O2-> 2/3Ga2O3+8/3Pd	-1572.97	-1553.77	-1534.77	-1515.95	-1497.28	-1478.76	-1460.37	-1442.09	-1423.92	-1405.85	-1387.86	-1369.96	-1352.13	-1334.38
2/3Ga2Pd5+O2-> 2/3Ga2O3+10/3Pd	-1820.44	-1800.71	-1781.18	-1761.83	-1742.64	-1723.59	-1704.67	-1685.87	-1667.17	-1648.58	-1630.07	-1611.64	-1593.3	-1575.02
4/21Ga7Pt3+O2-> 2/3Ga2O3+4/7Pt	-654.21	-635.18	-616.34	-597.69	-579.19	-560.83	-542.6	-524.48	-506.47	-488.56	-470.73	-452.99	-435.32	-417.72
2/3Ga2Pt+O2->	-236.95	-217.64	-198.55	-179.65	-160.91	-142.32	-123.88	-105.55	-87.33	-69.22	-51.2	-33.27	-15.42	2.35

2/3Ga2O3+2/3Pt														
4/9Ga3Pt+O2-> 2/3Ga2O3+4/9Pt	-318.41	-299.73	-281.39	-263.36	-245.62	-228.12	-210.86	-193.8	-176.93	-160.24	-143.7	-127.31	-111.07	-94.95
4/9Ga3Pt5+O2-> 2/3Ga2O3+20/9Pt	-159.71	-140.55	-121.58	-102.8	-84.17	-65.7	-47.35	-29.11	-10.99	7.04	24.98	42.83	60.61	78.32
4/15Ga5Pt+O2-> 2/3Ga2O3+4/15Pt	-804.89	-785.47	-766.26	-747.22	-728.34	-709.6	-690.99	-672.5	-654.11	-635.82	-617.61	-599.49	-581.45	-563.47
4/9Ga3Pt2+O2-> 2/3Ga2O3+8/9Pt	-222.67	-203.66	-184.84	-166.21	-147.74	-129.4	-111.2	-93.11	-75.12	-57.23	-39.43	-21.71	-4.07	13.5
4/3GaPt3+O2-> 2/3Ga2O3+4Pt	-117.65	-98.53	-79.63	-60.94	-42.44	-24.1	-5.9	12.16	30.1	47.93	65.66	83.29	100.83	118.29
4/3GaPt+O2-> 2/3Ga2O3+4/3Pt	-1175.63	-1156.57	-1137.71	-1119.03	-1100.5	-1082.12	-1063.87	-1045.73	-1027.7	-1009.76	-991.91	-974.15	-956.46	-938.84
4/3GaPt2+O2-> 2/3Ga2O3+8/3Pt	-2018.56	-1999.26	-1980.16	-1961.24	-1942.48	-1923.86	-1905.36	-1886.99	-1868.72	-1850.54	-1832.46	-1814.45	-1796.53	-1778.67

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