Erratum: First-principles thermodynamic framework for the evaluation of thermochemical H₂O- or CO₂-splitting materials [Phys. Rev. B 80, 245119 (2009)]

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In our paper,[1] the heat of formation ΔH_f or Gibbs free energy of formation ΔG_f of carbon monoxide was omitted from several equations corresponding to the gas-splitting (GS) step of two-step thermochemical CO₂-splitting cycles. The omission is typographical in nature; the proper forms of these equations were used in creating the paper's figures and in drawing the paper's conclusions.

Equation (6b) should read

$$
\begin{aligned}
\Delta G_{\mathrm{GS},T_{\mathrm{GS}}} = {} & \Delta H_{f,T_{\mathrm{GS}}}^{\mathrm{MO}_x} + \Delta H_{f,T_{\mathrm{GS}}}^{\mathrm{CO}} - \Delta H_{f,T_{\mathrm{GS}}}^{\mathrm{MO}_{x-1}} - \Delta H_{f,T_{\mathrm{GS}}}^{\mathrm{CO}_2} \\
& - T_{\mathrm{GS}}\big(S_{T_{\mathrm{GS}}}^{\mathrm{MO}_x} + S_{T_{\mathrm{GS}}}^{\mathrm{CO}} - S_{T_{\mathrm{GS}}}^{\mathrm{MO}_{x-1}} - S_{T_{\mathrm{GS}}}^{\mathrm{CO}_2}\big) \\
& \leqslant 0.
\end{aligned}
\tag{1}
$$

Equation (10b) should read

$$
\begin{aligned}
\Delta G_{\mathrm{GS},T_{\mathrm{GS}}} = {} & -\Delta H_{\mathrm{reduction}} + \Delta H_{f,T_{\mathrm{GS}}}^{\mathrm{CO}} - \Delta H_{f,T_{\mathrm{GS}}}^{\mathrm{CO}_2} \\
& - T_{\mathrm{GS}}\big(S_{T_{\mathrm{GS}}}^{\mathrm{CO}} - S_{T_{\mathrm{GS}}}^{\mathrm{CO}_2}\big) \leqslant 0.
\end{aligned}
\tag{2}
$$

Equation (11b) should read

$$
\begin{aligned}
\Delta T &= \frac{-2\big(\Delta G_{f,T_{\mathrm{GS}}}^{\mathrm{CO}_2} - \Delta G_{f,T_{\mathrm{GS}}}^{\mathrm{CO}}\big) - T_{\mathrm{GS}}\Delta S}{S_{T_{\mathrm{TR}}}^{\mathrm{O}_2}} \approx \frac{-2\big(\Delta G_{f,T_{\mathrm{GS}}}^{\mathrm{CO}_2} - \Delta G_{f,T_{\mathrm{GS}}}^{\mathrm{CO}}\big)}{S_{T_{\mathrm{TR}}}^{\mathrm{O}_2}} \\
&\Rightarrow S_{T_{\mathrm{TR}}}^{\mathrm{O}_2}\Delta T \approx -2\big(\Delta G_{f,T_{\mathrm{GS}}}^{\mathrm{CO}_2} - \Delta G_{f,T_{\mathrm{GS}}}^{\mathrm{CO}}\big).
\end{aligned}
\tag{3}
$$

In an unrelated typographical error, the text below (11b) should state that the ΔS term is roughly a 6% fraction of the numerator for both H₂O and CO₂ splitting, assuming TR occurs at 2000 K and GS occurs at 1000 K.

Equation (14b) should read

$$
\begin{aligned}
\Delta G_{\mathrm{GS},T_{\mathrm{GS}}} = {} & -\Delta H_{\mathrm{reduction}} + \Delta H_{f,T_{\mathrm{GS}}}^{\mathrm{CO}} - \Delta H_{f,T_{\mathrm{GS}}}^{\mathrm{CO}_2} \\
& - T_{\mathrm{GS}}\big(-\Delta S_{\mathrm{reduction}} + S_{T_{\mathrm{GS}}}^{\mathrm{CO}} - S_{T_{\mathrm{GS}}}^{\mathrm{CO}_2}\big) \\
& \leqslant 0.
\end{aligned}
\tag{4}
$$

Equation (15b) should read

$$
\Delta T = \frac{-2\big(\Delta G_{f,T_{\mathrm{GS}}}^{\mathrm{CO}_2} - \Delta G_{f,T_{\mathrm{GS}}}^{\mathrm{CO}}\big) - T_{\mathrm{GS}}\Delta S}{S_{T_{\mathrm{TR}}}^{\mathrm{O}_2} + 2\Delta S_{\mathrm{reduction}}}.
\tag{5}
$$

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[1]B. Meredig and C. Wolverton, Phys. Rev. B **80**, 245119 (2009).