

# Supplementary Information

## **Economic and environmental competitiveness of multiple hydrogen production pathways in China**

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## Supplementary Note 1. Optimization model of water electrolysis hydrogen production systems

### System 1: the grid hydrogen production system

#### Optimization objective

$$LCOH_{WE1} = \frac{C_{inv,WE1} + C_{om,WE1} + C_{grid,WE1} + C_{c,WE1}}{\sum_{n=1}^N \frac{H_{output}}{(1+r)^n}} \quad (1)$$

$$C_{inv,WE1} = c_{inv,EL} \cdot IC_{EL} \quad (2)$$

$$C_{om,WE1} = \sum_{n=1}^N \frac{c_{om,EL} \cdot IC_{EL}}{(1+r)^n} \quad (3)$$

$$C_{grid,WE1} = \sum_{n=1}^N \frac{\sum_{t=1}^{t=h} (c_{grid} \cdot EP_{grid}(t)) + c_{grid,fix1} \cdot EP_{grid,max} + \frac{c_{grid,fix2} \cdot EP_{grid,max}}{\cos \varphi}}{(1+r)^n} \quad (4)$$

$$C_{c,WE1} = c_c \cdot LCCE_{WE1} \quad (5)$$

#### Decision variables

The decision variable of configuration is the capacity of electrolyzer ( $IC_{EL}$ , kW). The decision variables of operation include the input power of the electrolyzer ( $EP_{EL}(t)$ , kW), the production of hydrogen of the electrolyzer ( $H_{EL}(t)$ , kg), the power purchased from the grid ( $EP_{grid}(t)$ , kW).

#### Constraints

##### (a) Equipment operation constraints

$$H_{EL}(t) \cdot LHV = \eta_{EL}(t) \cdot EP_{EL}(t) \quad (6)$$

$$0 \leq EP_{EL}(t) \leq IC_{EL} \quad (7)$$

$$0 \leq IC_{EL} \quad (8)$$

##### (b) Power purchase constraints

$$0 \leq EP_{grid}(t) \leq EP_{grid,max} \quad (9)$$

##### (c) Electricity balance constraints

$$EP_{grid}(t) = EP_{EL}(t) \quad (10)$$

##### (d) Hydrogen supply reliability constraints

$$H_{EL}(t) = \frac{H_{output}}{h} \quad (11)$$

## System 2: the hydrogen production system combined photovoltaic and grid

### Optimization objective

$$LCOH_{WE2} = \frac{C_{inv,WE2} + C_{om,WE2} + C_{grid,WE2} + C_{c,WE2}}{\sum_{n=1}^N \frac{H_{output}}{(1+r)^n}} \quad (12)$$

$$C_{inv,WE2} = c_{inv,PV} \cdot IC_{PV} + c_{inv,EL} \cdot IC_{EL} \quad (13)$$

$$C_{om,WE2} = \sum_{n=1}^N \frac{c_{om,PV} \cdot IC_{PV} + c_{om,EL} \cdot IC_{EL}}{(1+r)^n} \quad (14)$$

$$C_{grid,WE3} = \sum_{n=1}^N \frac{\sum_{t=1}^{t=h} (c_{grid} \cdot EP_{grid}(t)) + c_{grid,fix1} \cdot EP_{grid,max} + \frac{c_{grid,fix2} \cdot EP_{grid,max}}{\cos \varphi}}{(1+r)^n} \quad (15)$$

$$C_{c,WE1} = c_c \cdot LCCE_{WE2} \quad (16)$$

### Decision variables

The decision variables of configuration are the capacity of photovoltaic panels ( $IC_{PV}$ , kW) and the capacity of electrolyzer ( $IC_{EL}$ , kW). The decision variables of operation include the input power of the electrolyzer ( $EP_{EL}(t)$ , kW), the production of hydrogen of the electrolyzer ( $H_{EL}(t)$ , kg), the power purchased from the grid ( $EP_{grid}(t)$ , kW).

### Constraints

(a) Equipment operation constraints

$$EP_{PV}(t) = IC_{PV} \cdot EP_{PV,0}(t) \quad (17)$$

$$0 \leq IC_{PV} \quad (18)$$

$$H_{EL}(t) \cdot LHV = \eta_{EL}(t) \cdot EP_{EL}(t) \quad (19)$$

$$0 \leq EP_{EL}(t) \leq IC_{EL} \quad (20)$$

$$0 \leq IC_{EL} \quad (21)$$

(b) Power purchase constraints

$$0 \leq EP_{grid}(t) \leq EP_{grid,max} \quad (22)$$

(c) Electricity balance constraints

$$EP_{PV}(t) + EP_{grid}(t) = EP_{EL}(t) \quad (23)$$

(d) Hydrogen supply reliability constraints

$$H_{EL}(t) = \frac{H_{output}}{h} \quad (24)$$

## System 4: the off-grid hydrogen production system

### Optimization objective

$$LCOH_{WE4} = \frac{C_{inv,WE4} + C_{om,WE4} + C_{c,WE4}}{\sum_{n=1}^N \frac{H_{output}}{(1+r)^n}} \quad (25)$$

$$C_{inv,WE4} = c_{inv,PV} \cdot IC_{PV} + c_{inv,EL} \cdot IC_{EL} + c_{inv,EES} \cdot IC_{EES} + c_{inv,HST} \cdot IC_{HST} + c_{inv,com} \cdot IC_{com} \quad (26)$$

$$C_{om,WE4} = \sum_{n=1}^N \frac{c_{om,PV} \cdot IC_{PV} + c_{om,EL} \cdot IC_{EL} + c_{om,EES} \cdot IC_{EES} + c_{om,HST} \cdot IC_{HST} + c_{om,com} \cdot IC_{com}}{(1+r)^n} \quad (27)$$

$$C_{c,WE4} = c_c \cdot LCCE_{WE4} \quad (28)$$

### Decision variables

The decision variables of configuration include the capacity of photovoltaic panels ( $IC_{PV}$ , kW), the capacity of electrolyzer ( $IC_{EL}$ , kW), the capacity of compressor ( $IC_{com}$ , kW), and the capacity of electricity energy storage ( $IC_{EES}$ , kWh), the capacity of the hydrogen storage tank ( $IC_{HST}$ , kg). The decision variables of operation include the input power of the electrolyzer ( $EP_{EL}(t)$ , kW), the production of hydrogen of the electrolyzer ( $H_{EL}(t)$ , kg), the power consumption of the compressor ( $EP_{com}(t)$ , kW), the charging power of the electricity energy storage ( $EP_{EES,im}(t)$ , kW), the discharging power of the electricity energy storage ( $EP_{EES,ex}(t)$ , kW), hydrogen storage of the hydrogen storage tank ( $H_{HST,im}(t)$ , kg), hydrogen release of the hydrogen storage tank ( $H_{HST,ex}(t)$ , kg).

### Constraints

(a) Equipment operation constraints

$$EP_{PV}(t) = IC_{PV} \cdot EP_{PV,0}(t) \quad (29)$$

$$0 \leq IC_{PV} \quad (30)$$

$$H_{EL}(t) \cdot LHV = \eta_{EL}(t) \cdot EP_{EL}(t) \quad (31)$$

$$0 \leq EP_{EL}(t) \leq IC_{EL} \quad (32)$$

$$0 \leq IC_{EL} \quad (33)$$

$$EP_{com}(t) = EP_{com,0} \cdot H_{EL}(t) \cdot LHV \quad (34)$$

$$EP_{com}(t) \leq IC_{com} \quad (35)$$

$$\left\{ \begin{array}{l} E_{\text{EES}}(t+1) = E_{\text{EES}}(t)(1-\alpha) + (EP_{\text{EES,im}}(t)\eta_{\text{EES,im}} - EP_{\text{EES,ex}}(t)/\eta_{\text{EES,ex}})\Delta t \\ SOC_{\text{EES}}(t) = E_{\text{EES}}(t) / IC_{\text{EES}} \\ SOC_{\text{EES,min}} \leq SOC_{\text{EES}}(t) \leq SOC_{\text{EES,max}} \\ 0 \leq EP_{\text{EES,im}}(t) \leq EP_{\text{EES,im,max}} \\ 0 \leq EP_{\text{EES,ex}}(t) \leq EP_{\text{EES,ex,max}} \\ EP_{\text{EES,im}}(t) \cdot EP_{\text{EES,ex}}(t) = 0 \\ SOC_{\text{EES}}(t_{\text{start}}) = SOC_{\text{EES}}(t_{\text{end}}) \end{array} \right. \quad (36)$$

$$\left\{ \begin{array}{l} E_{\text{EES}}(t+1) = E_{\text{EES}}(t)(1-\alpha) + (EP_{\text{EES,im}}(t)\eta_{\text{EES,im}} - EP_{\text{EES,ex}}(t)/\eta_{\text{EES,ex}})\Delta t \\ SOC_{\text{EES}}(t) = E_{\text{EES}}(t) / IC_{\text{EES}} \\ SOC_{\text{EES,min}} \leq SOC_{\text{EES}}(t) \leq SOC_{\text{EES,max}} \\ 0 \leq EP_{\text{EES,im}}(t) \leq EP_{\text{EES,im,max}} \\ 0 \leq EP_{\text{EES,ex}}(t) \leq EP_{\text{EES,ex,max}} \\ EP_{\text{EES,im}}(t) \cdot EP_{\text{EES,ex}}(t) = 0 \\ SOC_{\text{EES}}(t_{\text{start}}) = SOC_{\text{EES}}(t_{\text{end}}) \end{array} \right. \quad (37)$$

(b) Electricity balance constraints

$$EP_{\text{PV}}(t) + EP_{\text{EES,ex}}(t) = EP_{\text{EES,im}}(t) + EP_{\text{EL}}(t) + EP_{\text{com}}(t) \quad (38)$$

(c) Hydrogen energy balance constraint

$$H_{\text{EL}}(t) = H_{\text{EL,out}}(t) + H_{\text{HST,im}}(t) \quad (39)$$

(d) Hydrogen supply reliability constraints

$$H_{\text{EL,out}}(t) + H_{\text{HST,ex}}(t) = \frac{H_{\text{output}}}{h} \quad (40)$$

## Supplementary Note 2. Data and parameters of optimization model

**Supplementary Table 1.** Technical and economic parameters of water electrolysis hydrogen production systems.

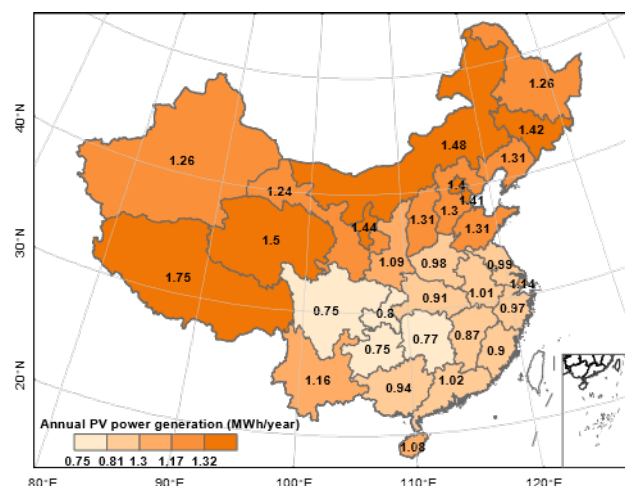
| Equipment                  | Parameter                                                                        | Symbol            | Value                 | Source     |
|----------------------------|----------------------------------------------------------------------------------|-------------------|-----------------------|------------|
| Photovoltaic panel         | Investment cost of photovoltaic panel (\$/kW)                                    | $c_{inv,PV}$      | 522                   | 1          |
|                            | Fixed operation and maintenance cost of photovoltaic panel (\$/kW-year)          | $c_{om,PV}$       | 52.2                  |            |
| Electrolyzer               | Investment cost of electrolyzer (Taking PEM electrolyzer as an example, \$/kW)   | $c_{inv,EL}$      | 1606.7                | 2          |
|                            | Fixed operation and maintenance cost of electrolyzer (\$/kW-year)                | $c_{om,EL}$       | 89.2                  |            |
|                            | Rated conversion efficiency of electrolyzer (%)                                  | $\eta_{EL}$       | 61.3                  |            |
| Electricity energy storage | Investment cost of electricity energy storage (\$/kWh)                           | $c_{inv,EES}$     | 344.2                 | 3, 4, 5, 6 |
|                            | Fixed operation and maintenance cost of electricity energy storage (\$/kWh-year) | $c_{om,EES}$      | 8.6                   |            |
|                            | Charging efficiency (%)                                                          | $\eta_{EES,im}$   | 0.945                 |            |
|                            | Discharging efficiency (%)                                                       | $\eta_{EES,ex}$   | 0.945                 |            |
|                            | The self-discharge rate (%/hour)                                                 | $\alpha$          | 0.002                 |            |
|                            | The maximum charging power (kW)                                                  | $EP_{EES,im,max}$ | $0.2 \times IC_{EES}$ |            |
|                            | The maximum discharging power (kW)                                               | $EP_{EES,ex,max}$ | $0.2 \times IC_{EES}$ |            |
|                            | The minimum state of charge                                                      | $SOC_{EES,min}$   | 0.2                   |            |
|                            | The maximum state of charge                                                      | $SOC_{EES,max}$   | 0.8                   |            |
| Hydrogen storage tank      | Investment cost of hydrogen storage tank (\$/kg)                                 | $c_{inv,EES}$     | 816.3                 | 6, 7, 8    |
|                            | Fixed operation and maintenance cost of hydrogen storage tank (\$/kg-year)       | $c_{om,EES}$      | 8.2                   |            |
|                            | The maximum rates of hydrogen import                                             | $H_{HST,im,max}$  | $IC_{HST}$            |            |
|                            | The maximum rates of hydrogen export                                             | $H_{HST,ex,max}$  | $IC_{HST}$            |            |
|                            | The minimum level of hydrogen (%)                                                | $LOH_{HST,min}$   | 0                     |            |
|                            | The maximum level of hydrogen (%)                                                | $LOH_{HST,max}$   | 100                   |            |
|                            | Pressure of hydrogen storage tank (bar)                                          | $p_{HST}$         | 200                   |            |
| Compressor                 | Investment cost of compressor (\$/kWh)                                           | $c_{inv,com}$     | 2666.3                | 6          |
|                            | Fixed operation and maintenance cost of compressor (\$/kWh-year)                 | $c_{om,com}$      | 106.6                 |            |

|         |                     |     |      |      |
|---------|---------------------|-----|------|------|
| General | System life (years) | $N$ | 20   | 2, 9 |
|         | Discount rate (%)   | $r$ | 3.85 |      |

**Supplementary Table 2.** Electricity prices of 31 provinces.

| Province            | Electricity price<br>(\$/kWh) | Capacitive demand electricity price |                                           |
|---------------------|-------------------------------|-------------------------------------|-------------------------------------------|
|                     |                               | Maximum demand<br>(\$/kW-year)      | Transformer<br>capacity (\$/kVA-<br>year) |
| Beijing (BJ)        | 0.0853                        | 79.3                                | 52.9                                      |
| Tianjin (TJ)        | 0.0957                        | 42.1                                | 28.1                                      |
| Shanghai (SH)       | 0.1056                        | 69.4                                | 46.3                                      |
| Chongqing (CQ)      | 0.0894                        | 59.5                                | 39.7                                      |
| Liaoning (LN)       | 0.0751                        | 54.5                                | 36.4                                      |
| Jilin (JL)          | 0.0868                        | 54.5                                | 36.4                                      |
| Heilongjiang (HL)   | 0.0827                        | 54.5                                | 36.4                                      |
| Inner Mongolia (IM) | 0.0660                        | 46.3                                | 31.4                                      |
| Shanxi (SX)         | 0.0679                        | 59.5                                | 39.7                                      |
| Hebei (HE)          | 0.0875                        | 57.9                                | 38.3                                      |
| Shandong (SD)       | 0.0941                        | 62.8                                | 46.3                                      |
| Shaanxi (SN)        | 0.0770                        | 51.2                                | 36.4                                      |
| Ningxia (NX)        | 0.0566                        | 49.6                                | 33.1                                      |
| Gansu (GS)          | 0.0593                        | 47.1                                | 31.4                                      |
| Qinghai (QH)        | 0.0519                        | 47.1                                | 31.4                                      |
| Xinjiang (XJ)       | 0.0542                        | 54.5                                | 43.0                                      |
| Tibet (XZ)          | 0.0930                        | 47.1                                | 31.4                                      |
| Sichuan (SC)        | 0.0565                        | 54.5                                | 36.4                                      |
| Yunnan (YN)         | 0.0614                        | 61.2                                | 44.6                                      |
| Guangxi (GX)        | 0.0949                        | 56.2                                | 45.5                                      |
| Guizhou (GZ)        | 0.0805                        | 52.9                                | 38.0                                      |
| Hunan (HN)          | 0.0959                        | 49.6                                | 33.1                                      |
| Guangdong (GD)      | 0.0956                        | 52.9                                | 38.0                                      |
| Fujian (FJ)         | 0.0819                        | 56.5                                | 37.7                                      |
| Zhejiang (ZJ)       | 0.0960                        | 66.1                                | 49.6                                      |
| Jiangxi (JX)        | 0.0951                        | 64.5                                | 43.0                                      |
| Anhui (AH)          | 0.0875                        | 66.1                                | 49.6                                      |
| Jiangsu (JS)        | 0.0899                        | 66.1                                | 49.6                                      |
| Hubei (HB)          | 0.0931                        | 62.8                                | 41.3                                      |
| Henan (HA)          | 0.0956                        | 46.3                                | 33.1                                      |
| Hainan (HI)         | 0.0863                        | 62.8                                | 43.0                                      |

Source: 35kV large-scale industrial electricity retail electricity price is the electricity price purchased from the power grid. The electricity price comes from the electricity price sales table of each provincial power grid company.



**Supplementary Figure 1.** Annual photovoltaic power generation in each province of China. The data of municipalities are directly obtained from PVWatts Calculator<sup>10</sup>. For different provinces, the average photovoltaic power generation data of the province is calculated in five cities distributed in different locations. For example, five representative cities, Jinan, Qingdao, Zaozhuang, Tai'an, and Weifang, are selected to calculate average photovoltaic power generation in Shandong province. Map Source: Standard Map Service of the Ministry of Natural Resources, People's Republic of China [Map Review Number: GS (2020) 4619].

**Supplementary Table 3.** Technical and economic parameters of hydrogen production from coal.

| Equipment | Unit investment cost (\$/kW H <sub>2</sub> ) | Annual operation and maintenance cost (\$/kW H <sub>2</sub> -year) | Efficiency (LHV)  | Carbon emission coefficient (kg CO <sub>2</sub> /kg H <sub>2</sub> ) |
|-----------|----------------------------------------------|--------------------------------------------------------------------|-------------------|----------------------------------------------------------------------|
| CG        | 2537.1 <sup>2</sup>                          | 126.9 <sup>2</sup>                                                 | 60 % <sup>2</sup> | 22.65 <sup>11</sup>                                                  |
| CG+CCUS   | 2642.1 <sup>2</sup>                          | 132.1 <sup>2</sup>                                                 | 58 % <sup>2</sup> | 10.59 <sup>11</sup>                                                  |

**Supplementary Table 4.** Technical and economic parameters of hydrogen production from natural gas<sup>3</sup>.

| Equipment | Unit investment cost (\$/kW H <sub>2</sub> ) | Annual operation and maintenance cost (\$/kW-year H <sub>2</sub> ) | fixed and cost (kWWh/kg H <sub>2</sub> ) | Electricity Use (kWWh/kg H <sub>2</sub> ) | Natural Gas Use (kg CH <sub>4</sub> /kg H <sub>2</sub> ) | Direct carbon emission coefficient (kg CO <sub>2</sub> /kg H <sub>2</sub> ) |
|-----------|----------------------------------------------|--------------------------------------------------------------------|------------------------------------------|-------------------------------------------|----------------------------------------------------------|-----------------------------------------------------------------------------|
| SMR       | 539.9                                        | 25.6                                                               |                                          | 0.65                                      | 3.53                                                     | 9.3                                                                         |
| SMR+CCUS  | 1313.9                                       | 57                                                                 |                                          | 2.04                                      | 3.75                                                     | 0.4                                                                         |

**Supplementary Table 5.** Natural gas prices of 31 provinces.

| Province            | Natural gas price (\$/m <sup>3</sup> ) |
|---------------------|----------------------------------------|
| Beijing (BJ)        | 0.395                                  |
| Tianjin (TJ)        | 0.489                                  |
| Shanghai (SH)       | 0.503                                  |
| Chongqing (CQ)      | 0.497                                  |
| Liaoning (LN)       | 0.500                                  |
| Jilin (JL)          | 0.421                                  |
| Heilongjiang (HL)   | 0.536                                  |
| Inner Mongolia (IM) | 0.179                                  |
| Shanxi (SX)         | 0.410                                  |
| Hebei (HE)          | 0.554                                  |
| Shandong (SD)       | 0.468                                  |
| Shaanxi (SN)        | 0.481                                  |
| Ningxia (NX)        | 0.463                                  |
| Gansu (GS)          | 0.398                                  |
| Qinghai (QH)        | 0.318                                  |
| Xinjiang (XJ)       | 0.310                                  |
| Tibet (XZ)          | 0.614                                  |
| Sichuan (SC)        | 0.579                                  |
| Yunnan (YN)         | 0.375                                  |
| Guangxi (GX)        | 0.565                                  |
| Guizhou (GZ)        | 0.512                                  |
| Hunan (HN)          | 0.450                                  |
| Guangdong (GD)      | 0.357                                  |
| Fujian (FJ)         | 0.584                                  |
| Zhejiang (ZJ)       | 0.579                                  |
| Jiangxi (JX)        | 0.537                                  |
| Anhui (AH)          | 0.573                                  |
| Jiangsu (JS)        | 0.444                                  |
| Hubei (HB)          | 0.511                                  |
| Henan (HA)          | 0.650                                  |
| Hainan (HI)         | 0.483                                  |

Source: <https://www.ceicdata.com.cn/zh-hans/china/gas-price-36-city><sup>12</sup>

**Supplementary Table 6.** Cost and carbon emissions of hydrogen production from industrial by-product.

| The type of industrial by-product hydrogen             | LCOH<br>(\$/kg H <sub>2</sub> ) | LCCE<br>(kg CO <sub>2</sub> /kg H <sub>2</sub> ) |
|--------------------------------------------------------|---------------------------------|--------------------------------------------------|
| Hydrogen by-production from light hydrocarbon cracking | 1.9-2.8                         | 8.9-12.9                                         |
| Hydrogen by-production from Chlor-alkali               | 1.8-2.8                         |                                                  |

|                                                                         |         |      |
|-------------------------------------------------------------------------|---------|------|
| Hydrogen by-production from Coke oven gas                               | 1.3-2.0 |      |
| Hydrogen by-production from ammonia synthesis, methanol synthesis, etc. | 2.0-3.1 |      |
| Average value                                                           | 2.2     | 10.9 |

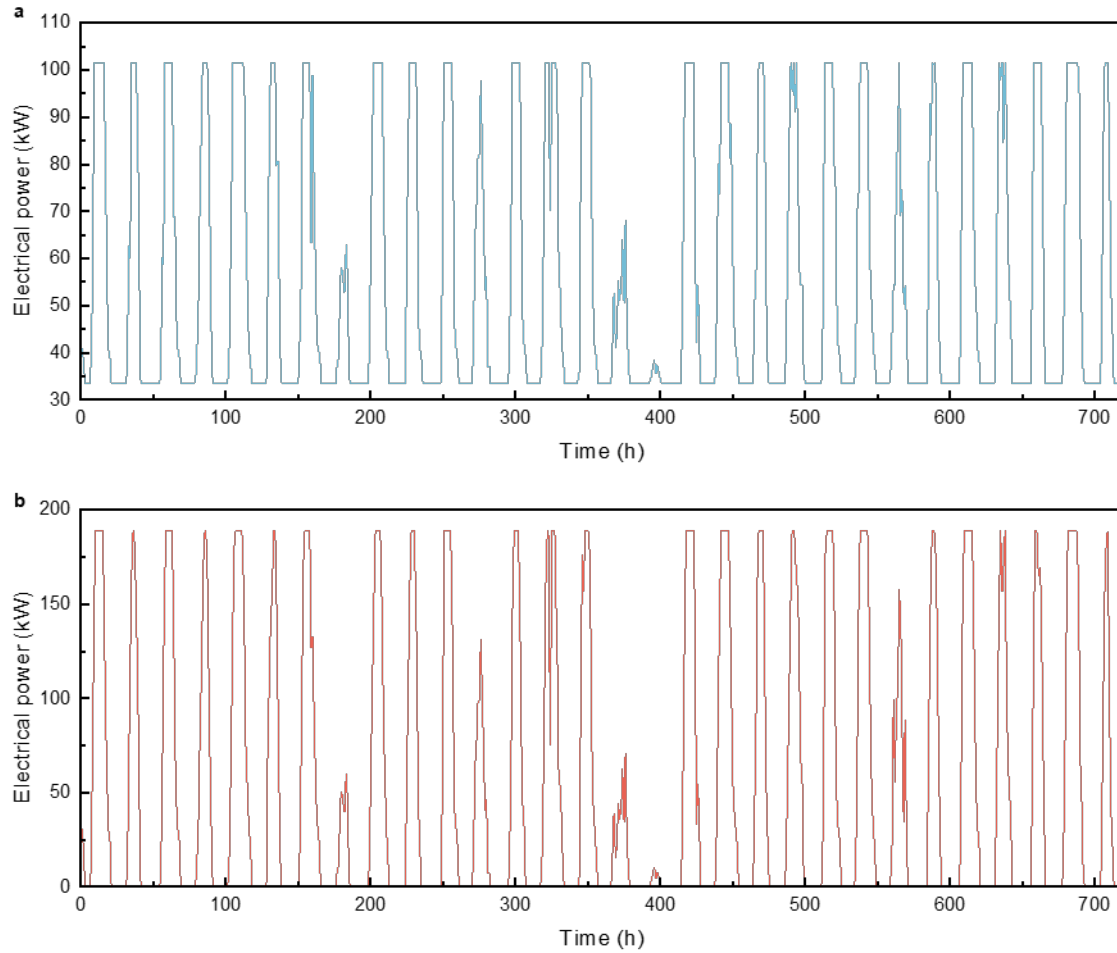
Source: Hydrogen Energy Industry Development Report of China 2020 <sup>13</sup>

**Supplementary Table 7.** Carbon emission factors of electricity purchase in 31 provinces.

| Province            | Carbon emission factor<br>(kg CO <sub>2</sub> /kWh) |
|---------------------|-----------------------------------------------------|
| Beijing (BJ)        | 0.615                                               |
| Tianjin (TJ)        | 0.841                                               |
| Shanghai (SH)       | 0.548                                               |
| Chongqing (CQ)      | 0.432                                               |
| Liaoning (LN)       | 0.91                                                |
| Jilin (JL)          | 0.839                                               |
| Heilongjiang (HL)   | 0.814                                               |
| Inner Mongolia (IM) | 1.000                                               |
| Shanxi (SX)         | 0.841                                               |
| Hebei (HE)          | 1.092                                               |
| Shandong (SD)       | 0.742                                               |
| Shaanxi (SN)        | 0.641                                               |
| Ningxia (NX)        | 0.872                                               |
| Gansu (GS)          | 0.46                                                |
| Qinghai (QH)        | 0.095                                               |
| Xinjiang (XJ)       | 0.749                                               |
| Tibet (XZ)          | 0.095                                               |
| Sichuan (SC)        | 0.117                                               |
| Yunnan (YN)         | 0.146                                               |
| Guangxi (GX)        | 0.526                                               |
| Guizhou (GZ)        | 0.42                                                |
| Hunan (HN)          | 0.487                                               |
| Guangdong (GD)      | 0.445                                               |
| Fujian (FJ)         | 0.489                                               |
| Zhejiang (ZJ)       | 0.532                                               |
| Jiangxi (JX)        | 0.616                                               |
| Anhui (AH)          | 0.763                                               |
| Jiangsu (JS)        | 0.695                                               |
| Hubei (HB)          | 0.316                                               |
| Henan (HA)          | 0.738                                               |
| Hainan (HI)         | 0.459                                               |

Source: China regional power grids carbon dioxide emission factors (2023) <sup>14</sup>

### Supplementary Note 3. Operation characteristics of water electrolysis hydrogen production systems in Beijing



**Supplementary Figure 2.** Hourly electric power of electrolyzer in a typical month. a and b are WE1 and WE2, respectively.

The degradation rate of the electrolyzer ( $D_{EL}$ ) is calculated as follows<sup>15</sup>.

$$D_{EL} = \frac{H_{sto,EL} + \frac{1}{h} \times \sum_{t=1}^{t=h} \left( \frac{EP_{EL}(t)}{IC_{EL}} \times (\sigma_{EL} - H_{sto,EL}) + k_{EL} f_{EL}(t)^2 \right)}{N_{EL}} \quad (41)$$

$$f_{EL}(t) = \frac{|EP_{EL}(t) - EP_{EL}(t-1)|}{IC_{EL}} \quad (42)$$

where,  $EP_{EL}$  is the electric power of the electrolyzer, kW.  $N_{EL}$  is the lifetime of the electrolyzer, year.  $H_{sto,EL}$ ,  $\sigma_{EL}$ ,  $k_{EL}$  are empirical coefficients related to the degradation rate, the proton exchange membrane (PEM) electrolyzer is taken as 0.35, 0.5,  $1 \times 10^{-5}$ , and the alkaline (ALK) electrolyzer is taken as 2, 10, 0.1, respectively.  $f_{EL}$  is the power volatility of the electrolyzer.

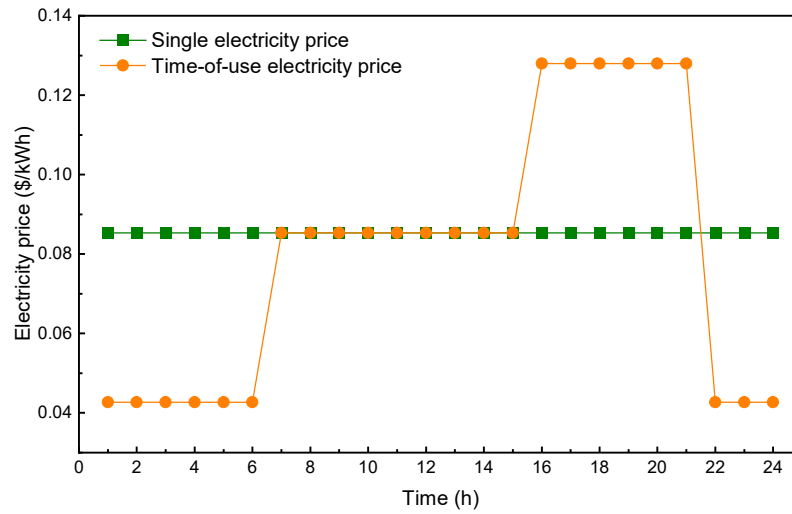
**Supplementary Table 8.** Full load operation time and degradation rate of four water electrolysis hydrogen production systems.

| System                        | WE1  | WE2  | WE3  | WE4  |
|-------------------------------|------|------|------|------|
| Full load operation hours (h) | 8760 | 8760 | 1679 | 1107 |
| Full load operation rate (%)  | 100  | 100  | 19.2 | 12.6 |
| Degradation rate (%)          | 2.5  | 2.5  | 2.2  | 1.9  |

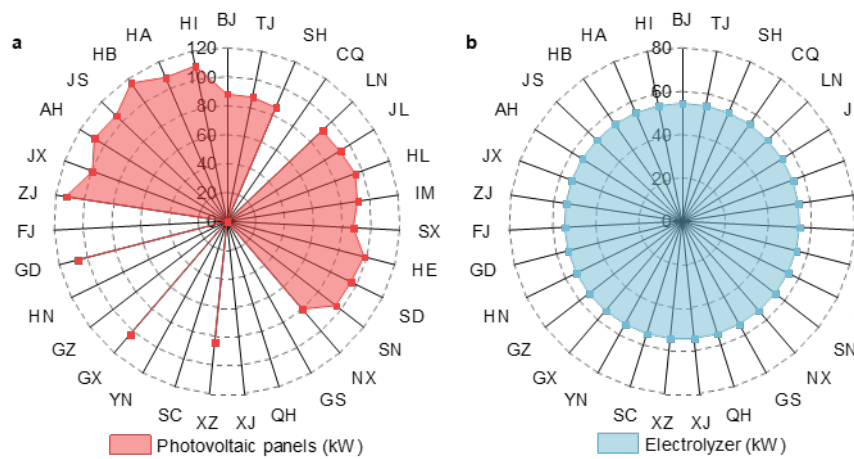
**Supplementary Table 9.** Comparison of electrolyzer degradation rates between constant power operation and dynamic operation. Taking WE4 as an example, the hydrogen production rate of the electrolyzer is 1kg/h in constant power operation.

| System               | Constant power operation | Dynamic operation |
|----------------------|--------------------------|-------------------|
| PEM electrolyzer (%) | 1.9                      | 1.9               |
| ALK electrolyzer (%) | 14.3                     | 15.9              |

# Supplementary Note 4. The setting and optimization results of time-of-use electricity price



**Supplementary Figure 3.** Single electricity price and time-of-use electricity price, taking Beijing as an example. On the basis of the single electricity price in each province, it fluctuates by 50% as the time-of-use electricity price in each province

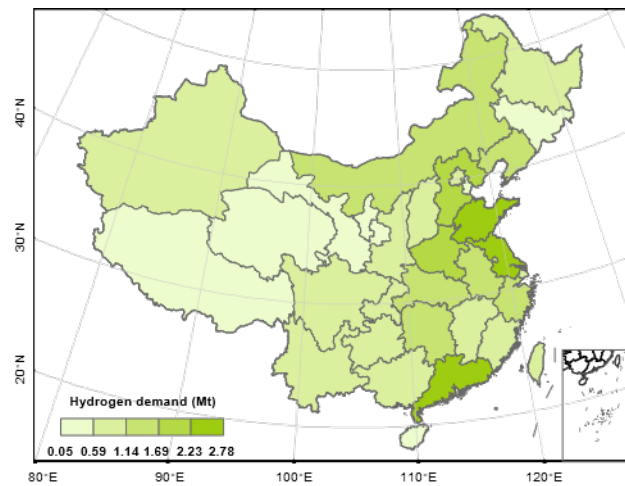


**Supplementary Figure 4.** Optimal configuration of WE2 system under time-of-use electricity price. a and b are the optimal capacities of the photovoltaic panels and the electrolyzer, respectively.



**Supplementary Figure 5.** Optimal configuration of WE3 system under time-of-use electricity price. a, b, c, d, and e are the optimal capacities of the photovoltaic panels, electrolyzer, electrical energy storage, hydrogen storage tank, and compressor, respectively.

### Supplementary Note 5. Distribution of hydrogen demand by province



**Supplementary Figure 6.** Distribution of hydrogen demand by province. Map  
Source: Standard Map Service of the Ministry of Natural Resources, People's  
Republic of China [Map Review Number: GS (2020) 4619].

## Supplementary Note 6. Setting parameters for the hydrogen production pathway for 2025-2050

**Supplementary Table 10.** Assumptions on economic and technical parameter of water electrolysis hydrogen production.

| Years                                                       | 2025 | 2030 | 2035  | 2040 | 2045 | 2050 | Source       |
|-------------------------------------------------------------|------|------|-------|------|------|------|--------------|
| Unit investment cost of PV (\$/kW)                          | 435  | 386  | 317   | 298  | 280  | 262  | <sup>1</sup> |
| Unit investment cost of electrolyzer (\$/kW)                | 1140 | 855  | 689   | 523  | 356  | 190  | <sup>2</sup> |
| Unit investment cost of electricity energy storage (\$/kWh) | 282  | 246  | 209   | 172  | 135  | 98   | <sup>4</sup> |
| Unit investment cost of hydrogen storage tank (\$/kg)       | 620  | 492  | 416   | 342  | 269  | 197  | <sup>6</sup> |
| Unit investment cost of compressor (\$/kW)                  | 2025 | 1606 | 1359  | 1116 | 877  | 640  | <sup>6</sup> |
| Conversion efficiency of electrolyzer (%)                   | 64   | 69   | 71.50 | 74   | 78.5 | 83   | <sup>2</sup> |

**Supplementary Table 11.** Assumptions on carbon price and coal price.

| Years | Carbon price (\$/t) | Coal price (\$/t) |
|-------|---------------------|-------------------|
| 2025  | 10.3                | 90.2              |
| 2030  | 16.5                | 93.8              |
| 2035  | 22.7                | 97.2              |
| 2040  | 28.9                | 100.7             |
| 2045  | 35.1                | 104.3             |
| 2050  | 41.3                | 107.7             |

Source: State Grid Energy Research Institution <sup>16</sup>

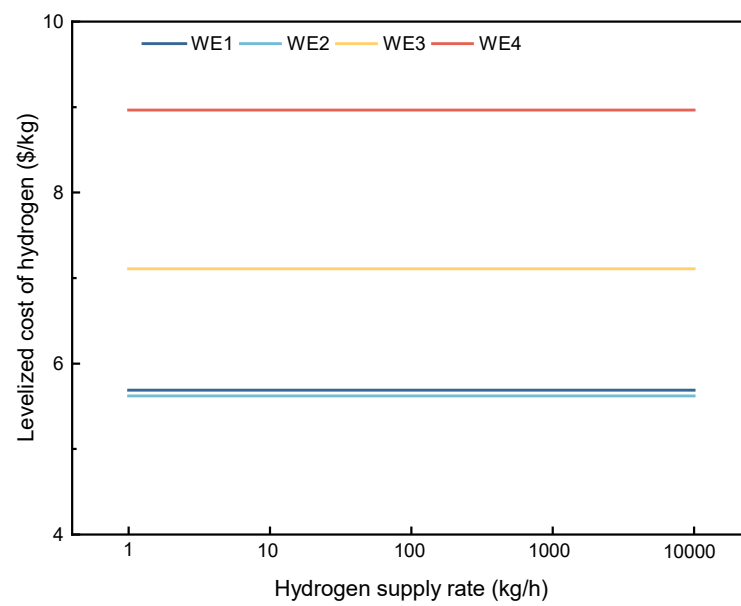
**Supplementary Table 12.** Assumptions on carbon emission factors of power grids in each province.

| Province            | 2020  | 2025  | 2030  | 2035  | 2040  | 2045  | 2050  |
|---------------------|-------|-------|-------|-------|-------|-------|-------|
| Beijing (BJ)        | 0.615 | 0.595 | 0.519 | 0.289 | 0.187 | 0.153 | 0.145 |
| Tianjin (TJ)        | 0.841 | 0.688 | 0.536 | 0.418 | 0.344 | 0.314 | 0.306 |
| Shanghai (SH)       | 0.548 | 0.333 | 0.325 | 0.281 | 0.251 | 0.237 | 0.233 |
| Chongqing (CQ)      | 0.432 | 0.363 | 0.256 | 0.179 | 0.136 | 0.120 | 0.115 |
| Liaoning (LN)       | 0.91  | 0.578 | 0.496 | 0.371 | 0.296 | 0.266 | 0.258 |
| Jilin (JL)          | 0.839 | 0.564 | 0.43  | 0.216 | 0.130 | 0.104 | 0.098 |
| Heilongjiang (HL)   | 0.814 | 0.654 | 0.599 | 0.504 | 0.440 | 0.412 | 0.404 |
| Inner Mongolia (IM) | 1.000 | 0.8   | 0.792 | 0.673 | 0.592 | 0.557 | 0.546 |
| Shanxi (SX)         | 0.841 | 0.707 | 0.7   | 0.598 | 0.528 | 0.497 | 0.489 |
| Hebei (HE)          | 1.092 | 0.736 | 0.683 | 0.544 | 0.455 | 0.418 | 0.408 |

|                |       |       |       |       |       |       |       |
|----------------|-------|-------|-------|-------|-------|-------|-------|
| Shandong (SD)  | 0.742 | 0.546 | 0.498 | 0.383 | 0.312 | 0.283 | 0.276 |
| Shaanxi (SN)   | 0.641 | 0.607 | 0.601 | 0.515 | 0.456 | 0.430 | 0.423 |
| Ningxia (NX)   | 0.872 | 0.724 | 0.665 | 0.459 | 0.345 | 0.302 | 0.291 |
| Gansu (GS)     | 0.46  | 0.443 | 0.407 | 0.279 | 0.209 | 0.183 | 0.176 |
| Qinghai (QH)   | 0.095 | 0.067 | 0.032 | 0.01  | 0.005 | 0.003 | 0.003 |
| Xinjiang (XJ)  | 0.749 | 0.720 | 0.713 | 0.573 | 0.483 | 0.445 | 0.435 |
| Tibet (XZ)     | 0.095 | 0.067 | 0.032 | 0.01  | 0.005 | 0.003 | 0.003 |
| Sichuan (SC)   | 0.117 | 0.104 | 0.075 | 0.04  | 0.025 | 0.020 | 0.019 |
| Yunnan (YN)    | 0.146 | 0.1   | 0.062 | 0.025 | 0.013 | 0.010 | 0.009 |
| Guangxi (GX)   | 0.526 | 0.336 | 0.334 | 0.279 | 0.242 | 0.226 | 0.222 |
| Guizhou (GZ)   | 0.42  | 0.398 | 0.276 | 0.204 | 0.161 | 0.145 | 0.140 |
| Hunan (HN)     | 0.487 | 0.453 | 0.409 | 0.312 | 0.253 | 0.229 | 0.222 |
| Guangdong (GD) | 0.445 | 0.369 | 0.332 | 0.276 | 0.239 | 0.223 | 0.218 |
| Fujian (FJ)    | 0.489 | 0.363 | 0.33  | 0.27  | 0.231 | 0.214 | 0.209 |
| Zhejiang (ZJ)  | 0.532 | 0.418 | 0.386 | 0.307 | 0.257 | 0.236 | 0.230 |
| Jiangxi (JX)   | 0.616 | 0.474 | 0.436 | 0.354 | 0.301 | 0.278 | 0.272 |
| Anhui (AH)     | 0.763 | 0.755 | 0.694 | 0.596 | 0.529 | 0.499 | 0.490 |
| Jiangsu (JS)   | 0.695 | 0.601 | 0.512 | 0.411 | 0.346 | 0.319 | 0.311 |
| Hubei (HB)     | 0.316 | 0.31  | 0.254 | 0.202 | 0.169 | 0.155 | 0.151 |
| Henan (HA)     | 0.738 | 0.599 | 0.49  | 0.389 | 0.325 | 0.298 | 0.291 |
| Hainan (HI)    | 0.459 | 0.326 | 0.224 | 0.115 | 0.070 | 0.057 | 0.053 |

Source: China regional power grids carbon dioxide emission factors (2023) <sup>14</sup>

### Supplementary Note 7. Sensitivity analysis of hydrogen supply rate



**Supplementary Figure 7.** Sensitivity analysis of hydrogen supply rate.

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