Electronic Supplementary Material (ESI) for Energy & Environmental Science.

Sector coupling via hydrogen to lower the cost of energy system decarbonization: Supplementary Information

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Supplementary Figures

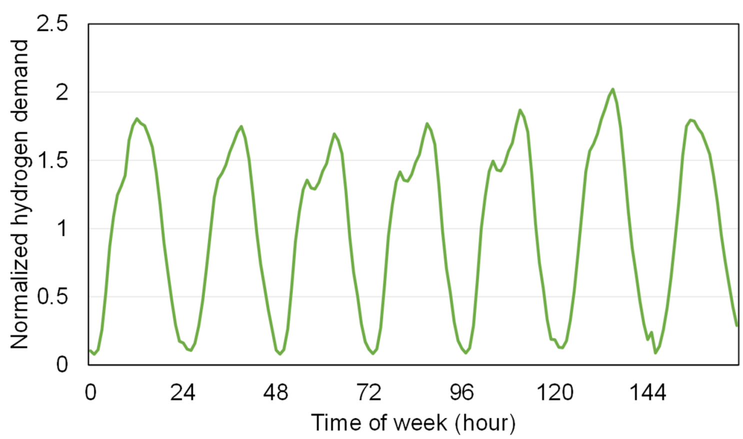

Figure S1. Hourly hydrogen refuelling profile normalized based on the mean

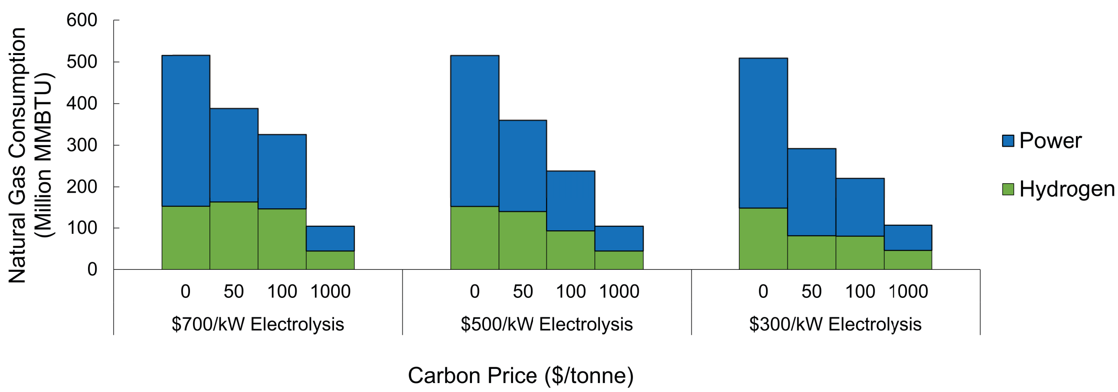

Figure S2. Natural gas consumption breakdowns in H_2 and power sectors.

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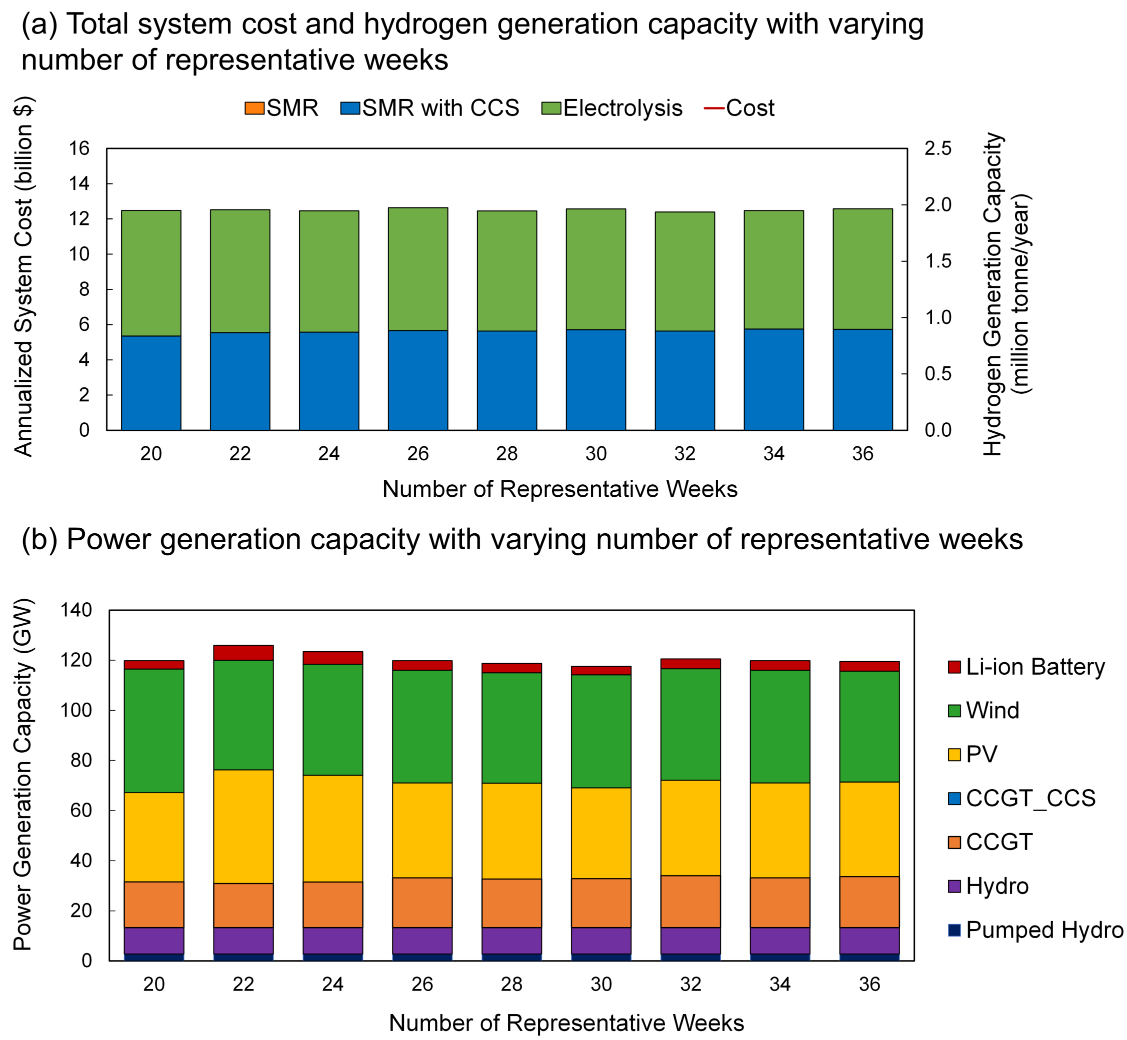

Figure S3. Total system cost and optimal generation and storage capacity mixes in the power and H_2 sectors with varying number of representative weeks, given \$100/tonne carbon price, 1 million tonne/year hydrogen demand, and \$300/kW electrolyzer cost. (a) Total system cost and H_2 generation capacity; (b) Power generation capacity. SMR: steam methane reformer; LH2: Liquid H_2; GH2: Gaseous H_2.

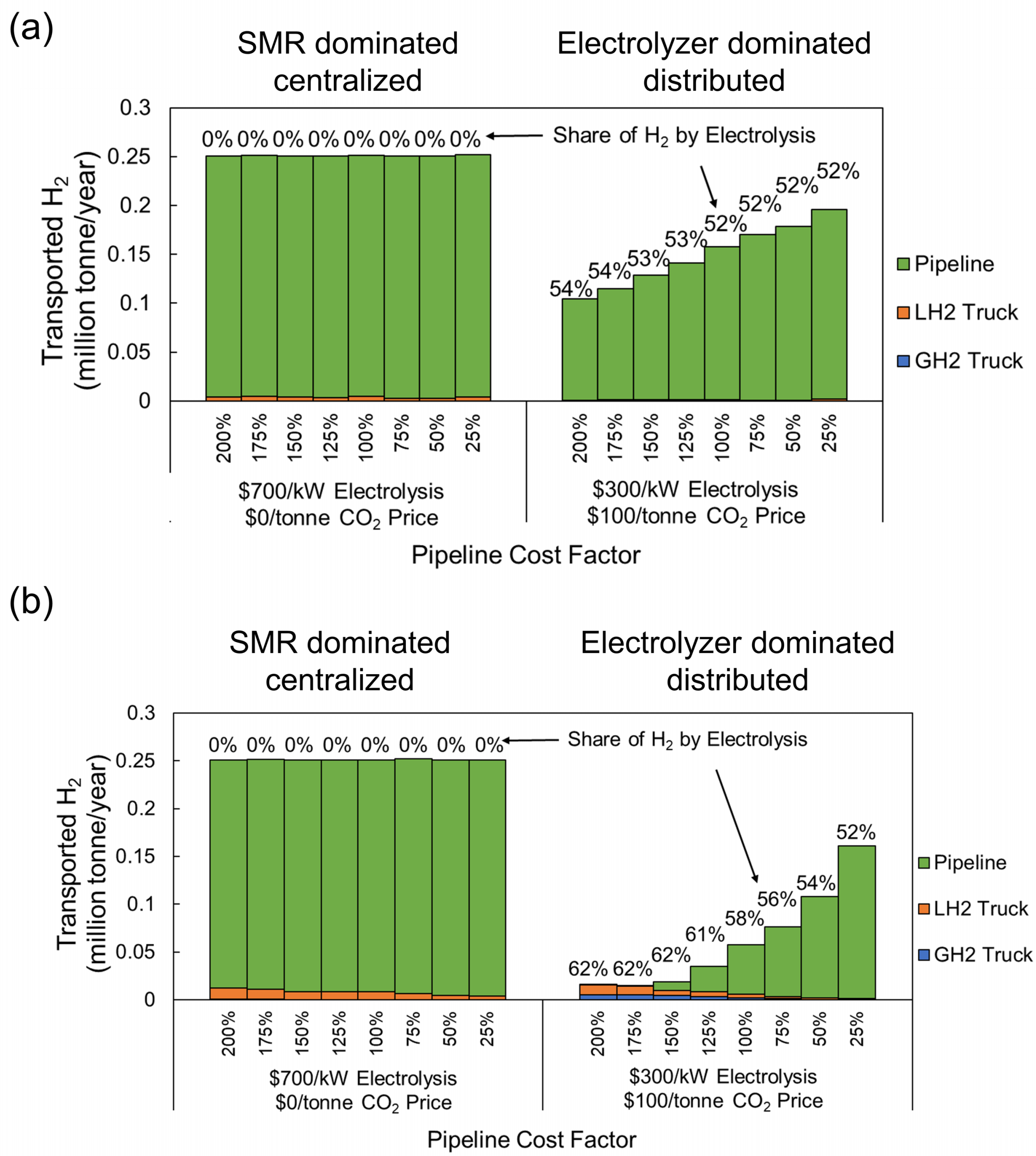

Figure S4. The amounts of transported H_2 per year via different transport modes under different pipeline cost scenarios and pipeline pressures. (a) 100 bar inlet pressure; (b) 80 bar inlet pressure. The baseline 100 bar pipeline parameters are shown in Table 3 (corresponding to 100% pipeline cost factor). For 80 bar pipeline, the baseline unit capacity is 4.3 tonne/hour, and the baseline capital cost is 1.58 million \$/unit. The H_2 demand is 1 million tonne/year. LH2: Liquid H_2; GH2: Gaseous H_2.

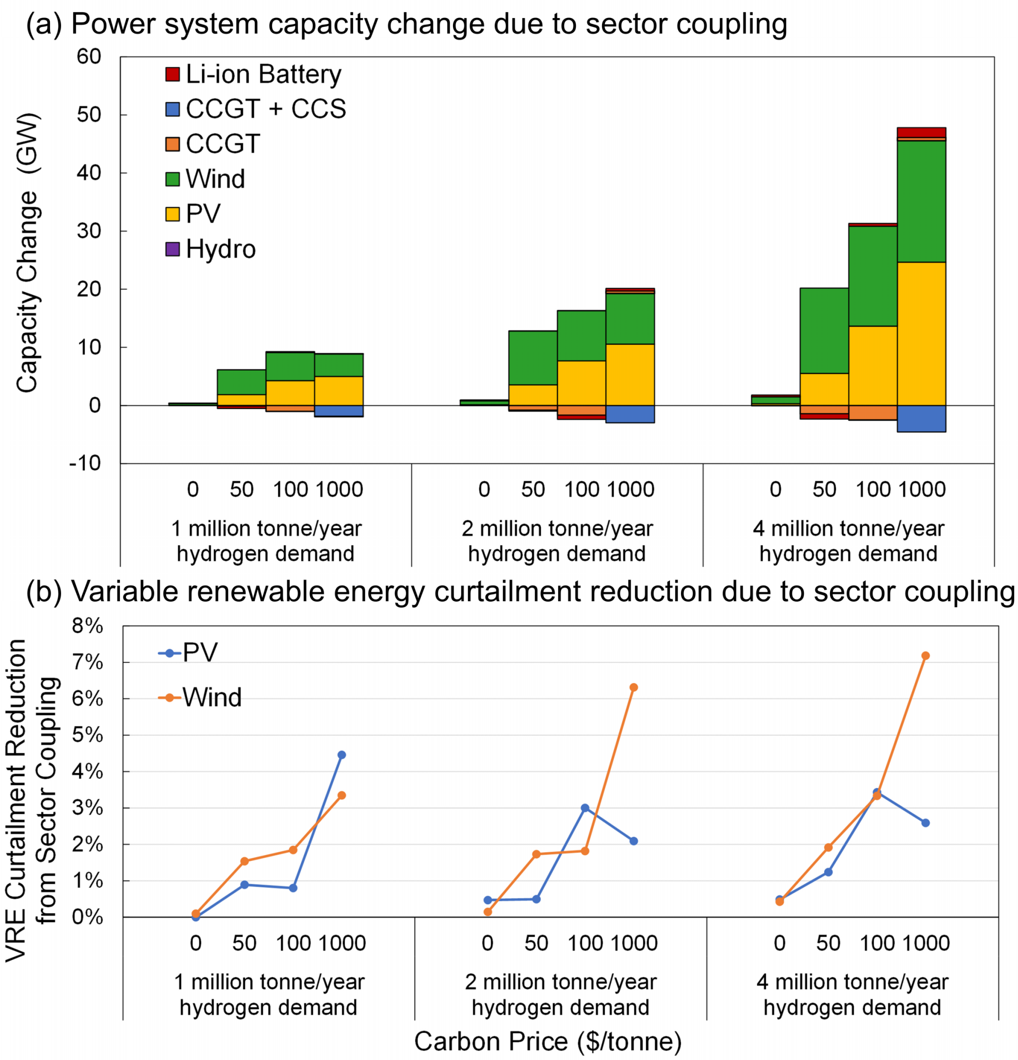

Figure S5. Differences in the optimal power system capacity mix and variable renewable energy (VRE) curtailment between energy systems with and without conversions between power to H_2 under various CO_2 price and FCEV penetration scenarios. (a) Differences in the optimal power system capacity mix; (b) Differences in the VRE curtailment. The carbon price varies from 0 to 1000 \$/tonne (upper x label). The hydrogen demand varies from 1 to 4 million tonne/year (lower x label). The capital cost of electrolyzer is assumed to be \$300/kW$_e$. In (b), the VRE curtailment reductions are calculated as the differences in the curtailment percentages between energy systems with and without conversions between power to H_2 in each CO_2 price and FCEV penetration scenario.

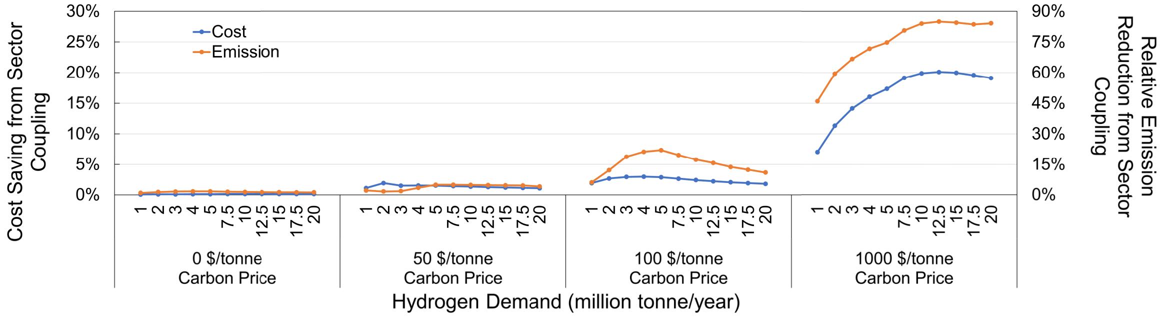

Figure S6. Differences in the total system cost and CO2 emission between energy systems with and without conversions between power to H_2 under various CO_2 price and hydrogen demand scenarios. The hydrogen demand varies from 1 to 20 million tonne/year (upper x label). The carbon price varies from 0 to 1000 $/tonne (lower x label). The capital cost of electrolyzer is assumed to be $300/kW$_e$. The cost savings are shown as percentages of the total system costs in each CO_2 price and hydrogen demand scenario, while the emission reductions are shown as percentages of the CO_2 emission in the case with $0/tonne CO_2 and respective hydrogen demand level.

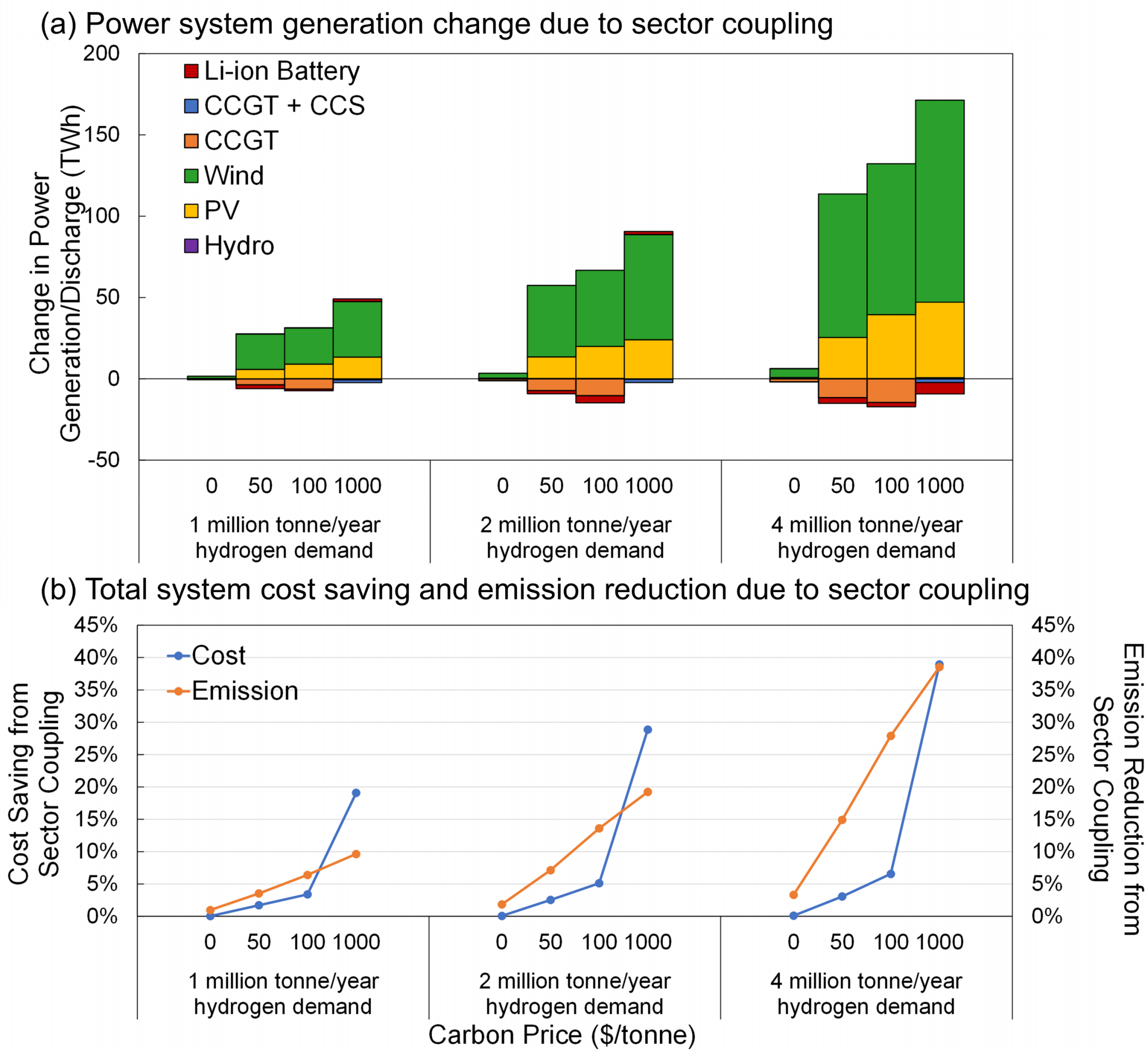

Figure S7. Differences in the optimal power system generation mix, total system cost, and CO_2 emission between energy systems with and without conversions between power to H_2 under various CO_2 price and hydrogen demand scenarios, considering non-combustion GHG emissions from natural gas. (a) Differences in the optimal power system generation mix; (b) Differences in the total system cost and CO_2 emission. The carbon price varies from 0 to 1000 $/tonne (upper x label). The hydrogen demand varies from 1 to 4 million tonne/year (lower x label). The capital cost of electrolyzer is assumed to be $300/kW$_e$. In (b), the cost savings are shown as percentages of the total system costs in each CO_2 price and hydrogen demand scenario, while the emission reductions are shown as percentages of the CO_2 emission in the case with $0/tonne CO_2, $300/kW electrolyzer, and 1 million tonne/year hydrogen demand.

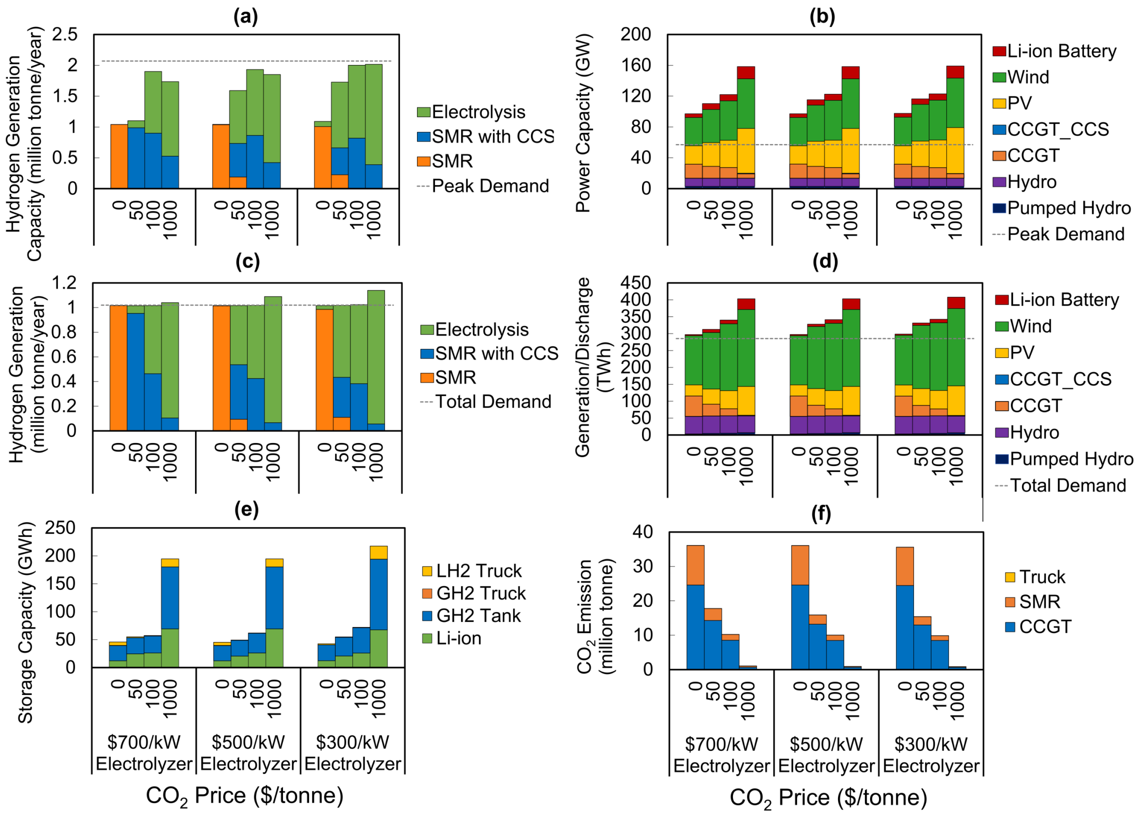

Figure S8. Optimal generation and storage capacity mixes and CO_2 emissions in the power and H_2 sectors under various CO_2 price and electrolysis cost scenarios in U.S. Northeast, considering non-combustion GHG emissions from natural gas. Technologies that are not cost-competitive are not shown. (a) H_2 generation capacity; (b) Power generation capacity; (c) H_2 generation per year; (d) Electricity generation or electrical storage energy discharge per year; (e) Chemical/electrochemical energy storage capacity in power and H_2 sectors; (f) CO_2 emissions in power and H_2 sectors. The hydrogen demand is 1 million tonne/year. The carbon price varies from 0 to 1000 $/tonne (upper x label). The electrolyzer cost varies from $700/kW to $300/kW (lower x label). SMR: steam methane reformer; LH2: Liquid H_2; GH2: Gaseous H_2.

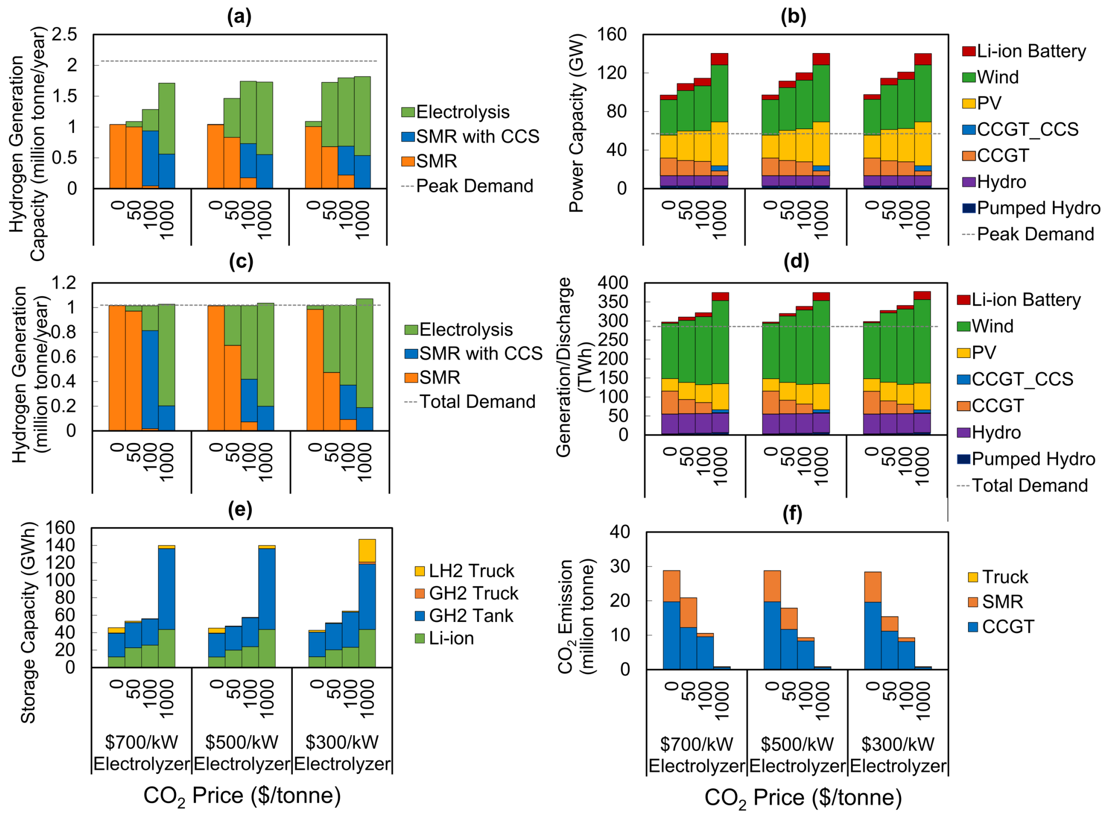

Figure S9. Optimal generation and storage capacity mixes and CO_2 emissions in the power and H_2 sectors under various CO_2 price and electrolysis cost scenarios in U.S. Northeast, given the current cost of SMR with CCS. (a) H_2 generation capacity; (b) Power generation capacity; (c) H_2 generation per year; (d) Electricity generation or electrical storage energy discharge per year; (e) Chemical/electrochemical energy storage capacity in power and H_2 sectors; (f) CO_2 emissions in power and H_2 sectors. The hydrogen demand is 1 million tonne/year. The carbon price varies from 0 to 1000 \$/tonne (upper x label). The electrolyzer cost varies from \$700/kW to \$300/kW (lower x label). The capital cost of SMR with CCS is \$1680/kW_{H_2}. SMR: steam methane reformer; LH2: Liquid H_2; GH2: Gaseous H_2.

Supplementary Tables

Table S1. Additional Parameters of the DOLPHYN model

Discount rate	5.4%
Power transmission expansion cost	1,600/MW-mile
Power transmission loss	1%/100 miles
Value of lost load (electricity)	\$20,000/MWh
Value of lost load (hydrogen)	\$1,000/kg
Gas Price	\$5.4/MMBTU
CO_2 transportation and storage cost	\$20/tonne

Table S2. Parameters of Existing power transfer capacity (High Voltage AC) between various model zones. Zone 7 represents Canada. For each line, transmission losses are computed based on 1% per 100 miles loss factor (Table S1) and the distance between the centroid of the two zones

Line	Max Power Flow (MW)	Line Distance (km)	Transmission Loss Percentage
Zone 1-2	2000	317	3.17%
Zone 2-3	2950	199	1.99%
Zone 3-4	760	99	0.99%
Zone 4-5	1528	216	2.16%
Zone 3-5	600	158	1.58%
Zone 2-5	800	179	1.79%
Zone 5-6	5400	186	1.86%
Zone 2-6	150	340	3.40%
Zone 6-7	2600	0	2.40%
Zone 2-7	1650	0	2.40%
Zone 1-7	800	0	2.40%

Table S3. Inter-Zone Distances of the Six Zones in the U.S. Northeast for Trucks and Pipelines (mile).

Zone	**1**	**2**	**3**	**4**	**5**	**6**
1	0	317	504	602	487	608
2	317	0	199	297	179	340
3	504	199	0	99	158	333
4	602	297	99	0	216	358
5	487	179	158	216	0	186
6	608	340	333	358	186	0

Table S4. Power capacities for the results of Figure 3. All capacity units are GW.

Electrolyser Cost	Carbon Price	Pumped Hydro	Hydro	PV	Wind	Nuclear	CCGT	CCGT w/ CCS	OCGT	Li-ion Battery
$700/kW	0 $/tonne	2.8	10.5	23.8	36.7	0	18.4	0	6.9	4.9
	50 $/tonne	2.8	10.5	30.5	41.8	0	15.9	0	5.6	7.3
	100 $/tonne	2.8	10.5	30.8	46.1	0	15.0	0	5.1	8.1
	1000 $/tonne	2.8	10.5	44.6	58.6	0	4.8	5.2	0	12.5
$500/kW	0 $/tonne	2.8	10.5	23.8	36.7	0	18.4	0	6.9	4.9
	50 $/tonne	2.8	10.5	30.5	43.2	0	15.9	0	5.8	6.8
	100 $/tonne	2.8	10.5	33.4	49.3	0	14.5	0	4.6	8.1
	1000 $/tonne	2.8	10.5	44.9	58.2	0	4.7	5.2	0	12.3
$300/kW	0 $/tonne	2.8	10.5	23.8	37.0	0	18.4	0	6.8	4.9
	50 $/tonne	2.8	10.5	32.2	45.8	0	15.7	0	5.3	7.0
	100 $/tonne	2.8	10.5	34.0	49.9	0	14.4	0	4.4	8.0
	1000 $/tonne	2.8	10.5	44.5	57.9	0	4.8	5.2	0	11.8

Table S5. Capacity factors of power sector infrastructures for the results of Figure 3.

Electrolyser Cost	Carbon Price	Pumped Hydro	Hydro	PV	Wind	Nuclear	CCGT	CCGT w/ CCS	OCGT	Li-ion Battery
$700/kW	0 $/tonne	0.13	0.56	0.16	0.45	0	0.38	0	0.01	0.08
	50 $/tonne	0.18	0.56	0.17	0.44	0	0.27	0	0.01	0.13
	100 $/tonne	0.19	0.56	0.17	0.44	0	0.23	0	0.01	0.15
	1000 $/tonne	0.25	0.55	0.17	0.42	0	0.02	0.15	0	0.20
$500/kW	0 $/tonne	0.13	0.56	0.16	0.45	0	0.37	0	0.01	0.08
	50 $/tonne	0.17	0.56	0.17	0.45	0	0.26	0	0.01	0.12
	100 $/tonne	0.19	0.56	0.17	0.45	0	0.19	0	0.01	0.14
	1000 $/tonne	0.25	0.55	0.18	0.43	0	0.02	0.15	0	0.20
$300/kW	0 $/tonne	0.13	0.56	0.16	0.45	0	0.37	0	0.01	0.08
	50 $/tonne	0.15	0.56	0.17	0.45	0	0.25	0	0.01	0.10
	100 $/tonne	0.18	0.56	0.17	0.45	0	0.18	0	0.01	0.14
	1000 $/tonne	0.26	0.55	0.18	0.43	0	0.02	0.15	0	0.21