

Supporting information

An Air Chargeable Hydrogen Battery by Reversible Electrochemical Trapping of the Protons

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Results and discussion:

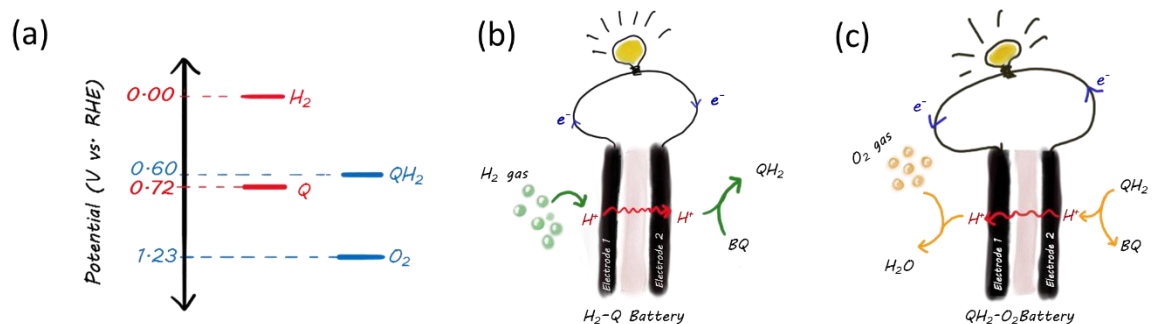


Figure S1: (a) Single electrode potentials of BQ and QH₂ electrodes with respect to H₂/H⁺ and O₂/H₂O half-cell reactions. Schematic representation of reactions occurring at the (b) H₂-BQ battery and (c) QH₂-O₂ battery.

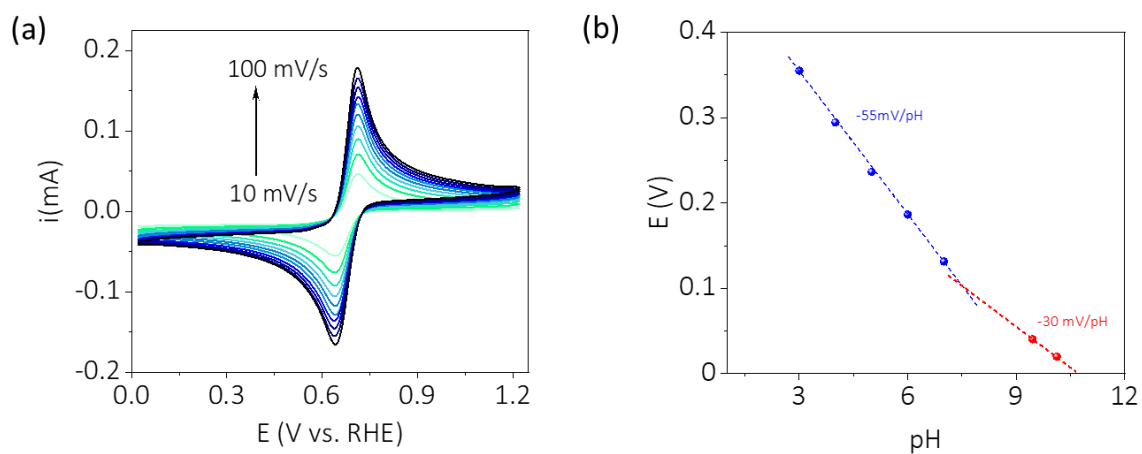


Figure S2: (a) Cyclic voltammogram of benzoquinone (BQ) in 0.5 M H₂SO₄ on a glassy carbon electrode at different scan rates. (b) pH vs. potential (Pourbaix diagram) of 5 mM benzoquinone at different pH.

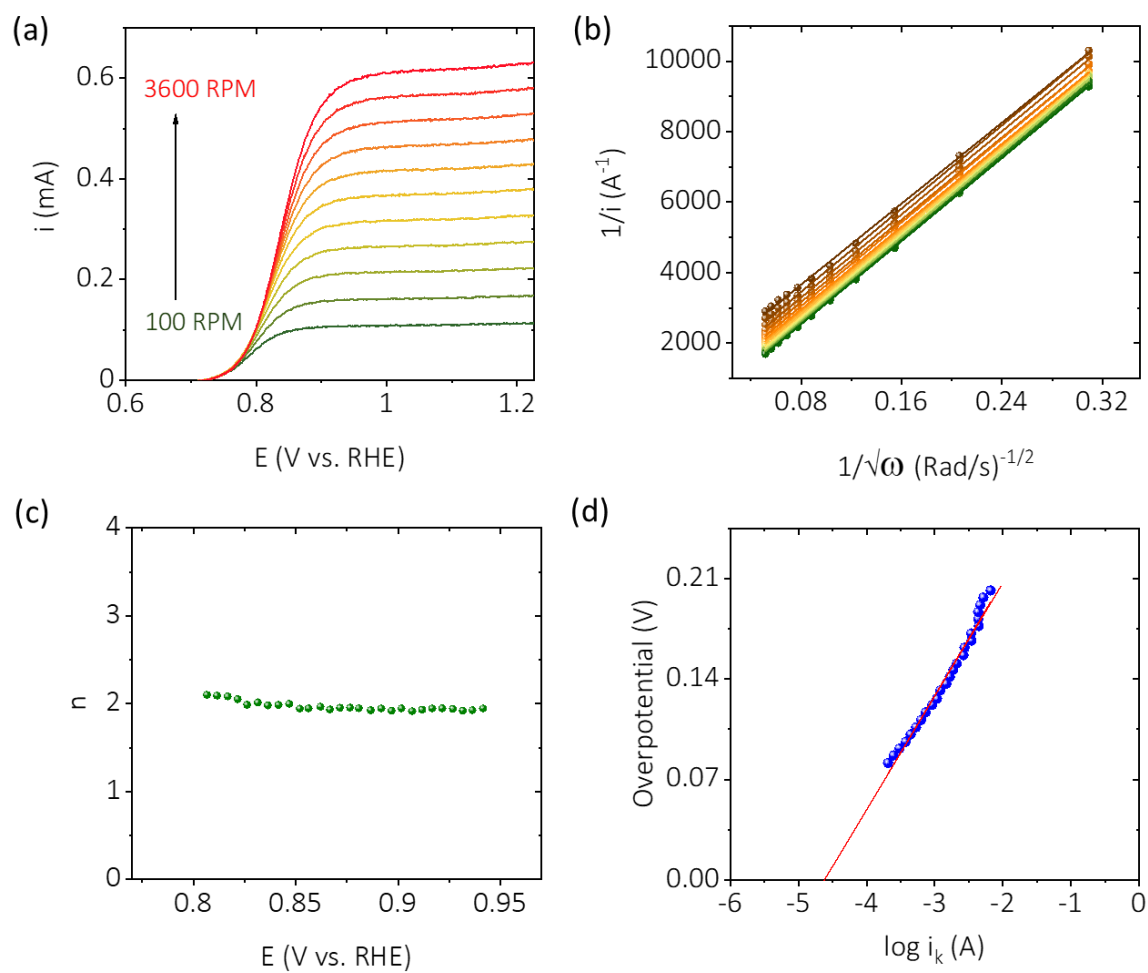


Figure S3: (a) RDE of QH₂ oxidation. (b) Koutecky-Levich plots for QH₂ oxidation. (c) Number of electrons (n) involved during QH₂ oxidation. (d) Overpotential vs. $\log i_k$ for QH₂ oxidation.

Table S1: Electrochemical parameters extracted from RRDE and Koutecky-Levich plot.

Species	No: of electrons	β	Rate constant (cm/s)
Benzoquinone/Hydroquinone	2.03	0.42	$1.3 \cdot 10^{-4}$

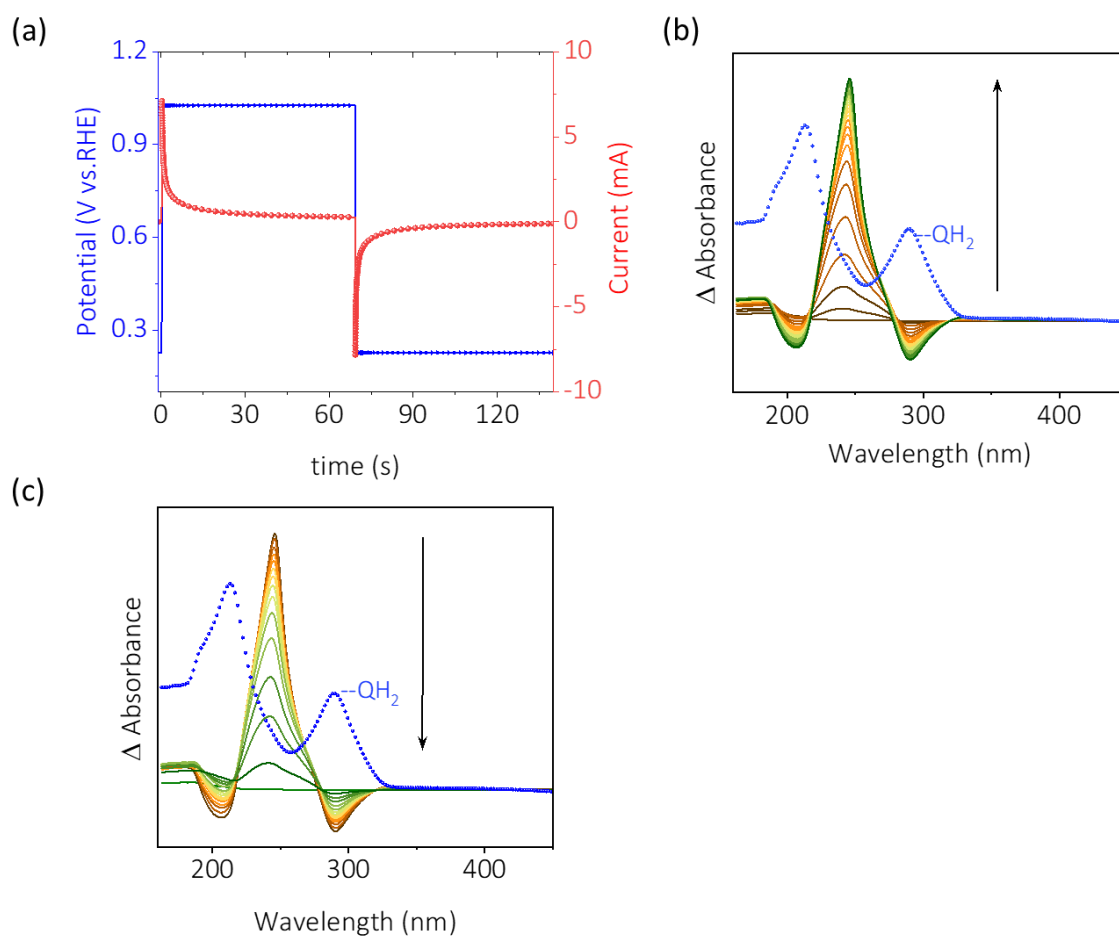


Figure S4: In-situ UV-Vis spectroelectrochemistry data for the redox reaction of benzoquinone. (a) Chronoamperometry, (b) the potential dependent spectra acquired during the oxidation scan and (c) during the reduction scan.

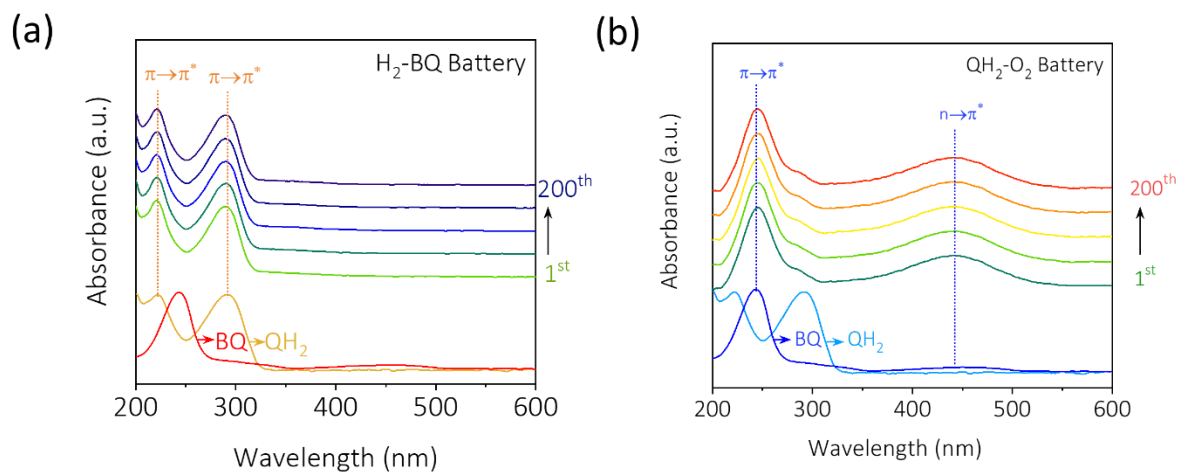


Figure S5: UV-Vis spectra (a) H₂-Q battery cathode and (b) QH₂-O₂ battery anode during different discharge cycles.

Table S2: Battery discharge capacity

	Discharge capacity in mAh/g	
	H ₂ -BQ Battery	QH ₂ -O ₂ Battery
1 st cycle	364.69	364.54
10 th cycle	364.14	362.97
50 th cycle	355.13	353.70
100 th cycle	343.24	342.00
200 th cycle	330.44	329.41

Table S3: Calculation of cumulative capacity

	Cumulative discharge capacity (mAh/g)	
	H ₂ -BQ Battery	QH ₂ -O ₂ Battery
1 st – 10 th cycle	3644.15	3637.55
11 th – 50 th cycle	14385.44	14333.40
51 th -100 th cycle	17459.17	17392.55
101 th – 200 th cycle	33684.15	33570.00
Total	69172.91	68933.50

Calculation S1:

Amount(g) of BQ used in 100 ml of 0.1 M solution : $\frac{108.1 \times 0.1 \times 100}{1000} = 1.081 \text{ g}$

No: of moles of BQ : $\frac{1.081}{108.1} = 0.01 \text{ moles}$

Electric charge : $0.01 \times 2 = 0.02 \text{ F}$

Amount of hydrogen required : 0.01 moles

Amount of oxygen required : 0.005 moles

Calculation S2:

First discharge capacity of H₂-BQ battery: 364.69 mAh/g

Cumulative capacity of H₂-BQ battery after 200 cycles: 69172.91 mAh/g

Cumulative capacity of QH₂-O₂ battery after 200 cycles: 68933.5 mAh/g

Cumulative capacity of the battery in total: 138106.41 mAh/g

Amount (g) of BQ required to achieve a capacity of 69172.91 mAh (Table S3) in primary battery configuration: $69172.91 / 364.69 = 189.67 \text{ g}$

Similarly, amount (g) of QH₂ required to achieve a capacity of 68933.5 mAh (Table S3) in primary battery configuration: $68933.50 / 364.54 = 189.09 \text{ g}$

Therefore, cumulative capacity during discharge and air charge processes = 378.76 g