Electronic Supplementary Information

Synthesis of mesoporous Fe$_3$Si aerogel as a photo-thermal material for highly efficient and stable corrosive-water evaporation

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Figure S1. The emission spectrum of xenon lamp provided by perfectlight Co., Ltd.
Figure S2. (a) Nitrogen adsorption and desorption isotherm, (b) pore size distribution (c) ultraviolet-Visible-Near Infrared absorption spectrum, (d) Fe 2p XPS spectrum of Fe-doped SiO$_2$ aerogel.
Figure S3. (a) HRTEM image of the interface between Fe$_3$Si crystal and amorphous SiO$_2$ in Fe$_3$Si aerogel. (b) SEM image, (c) ultraviolet-visible-near infrared absorption spectrum, (d) XRD pattern of SiO$_2$ aerogel.
Figure S4. (a) XRD pattern, (b) SEM image, (c) ultraviolet-visible-near infrared absorption spectrum, (d) temperature-dependent total thermal conductivity of pure bulk Fe$_3$Si particles.
Figure S5. (a) Photograph of Fe$_3$Si aerogel loaded in a glass dish, (b) the corresponding infra-red (IR) image with the irradiation of 1 kW·m$^{-2}$ standard sunlight obtained by IR camera.
Figure S6. (a,b) Photographs and (c,d) corresponding top-view and side-view IR images of bulk Fe₃Si aerogel supported on melamine foam in solar-vapor desalination unit after 10 minutes of 1.0 kw·m⁻² sunlight illumination. (e) Photograph and (f) IR image of SiO₂ aerogel supported on melamine foam in solar-vapor desalination unit after 10 minutes of 1.0 kw·m⁻² sunlight illumination.
Figure S7. (a) Infrared (IR) image (obtained by IR camera) of hydrophobic Fe$_3$Si aerogel/melamine foam in solar-vapor desalination unit after 5 minutes of 1.0 kw·m$^{-2}$ sunlight illumination. (b) The seawater evaporation performance of hydrophobic Fe$_3$Si aerogel/melamine foam under 1.0 kw·m$^{-2}$ solar illumination.
Table S1. Water evaporation performance comparison of Fe$_3$Si aerogel/melamine foam and other excellent photothermal materials under sunlight irradiation. The sunlight intensity is around 1000 W·m$^{-2}$.

<table>
<thead>
<tr>
<th>Materials</th>
<th>Supports</th>
<th>Evaporation rate</th>
<th>ratio (η)</th>
<th>Refs</th>
</tr>
</thead>
<tbody>
<tr>
<td>PVA gel/PPy</td>
<td>none</td>
<td>3.2kg·m$^{-2}$·h$^{-1}$</td>
<td>8</td>
<td>1</td>
</tr>
<tr>
<td>Hollow carbon</td>
<td>none</td>
<td>1.45kg·m$^{-2}$·h$^{-1}$</td>
<td>2.9</td>
<td>2</td>
</tr>
<tr>
<td>GO and CNTs</td>
<td>GO/cellulose</td>
<td>1.25kg·m$^{-2}$·h$^{-1}$</td>
<td>3.125</td>
<td>3</td>
</tr>
<tr>
<td>graphene foam</td>
<td>none</td>
<td>1.4kg·m$^{-2}$·h$^{-1}$</td>
<td>3.5</td>
<td>4</td>
</tr>
<tr>
<td>Ti$_3$O$_3$</td>
<td>cellulose</td>
<td>1.32kg·m$^{-2}$·h$^{-1}$</td>
<td>2.6</td>
<td>5</td>
</tr>
<tr>
<td>Mg reduced TiO$_2$</td>
<td>SS mesh</td>
<td>0.8kg·m$^{-2}$·h$^{-1}$</td>
<td>1.8</td>
<td>6</td>
</tr>
<tr>
<td>Fe$_3$Si aerogel</td>
<td>none</td>
<td>2.08kg·m$^{-2}$·h$^{-1}$</td>
<td>6.71</td>
<td>This work</td>
</tr>
</tbody>
</table>

PVA: poly vinyl alcohol; PPy: polypyrrole; GO: graphene oxide; CNTs: carbon nanotubes; SS: stainless steel.
Figure S8. (a) Water evaporation rate under dark circumstances and (b) the corresponding calculated equivalent enthalpy in different conditions.

The calculation is in term of the equation below:

\[ U = \Delta H_1 \cdot m_1 = \Delta H_2 \cdot m_2 \] (eq1)

Where \( \Delta H_1 \) and \( m_1 \) were the evaporation enthalpy and water evaporation rate of pure water under dark circumstances.\(^1\) The different water evaporation cells was put in same dark room at same time under a temperature of 23 °C, and the value of \( \Delta H_1 \) was 2450 KJ·kg\(^{-1}\).
Table S2. The seawater evaporation performance comparison of Fe$_3$Si aerogel, bulk Fe$_3$Si supported on melamine foam and self-floated Fe$_3$Si aerogel (S-Fe$_3$Si aerogel)

<table>
<thead>
<tr>
<th>Materials</th>
<th>Water evaporation mass for 2 h (kg·m$^{-2}$)</th>
<th>Latent heat (kJ/kg)</th>
<th>Temperature increase of water $\Delta T$ (k)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe$_3$Si aerogel</td>
<td>4.16</td>
<td>1520</td>
<td>29</td>
</tr>
<tr>
<td>Bulk Fe$_3$Si</td>
<td>2.30</td>
<td>2215</td>
<td>22</td>
</tr>
<tr>
<td>S-Fe$_3$Si aerogel</td>
<td>1.49</td>
<td>2295</td>
<td>61</td>
</tr>
</tbody>
</table>

To assess the effect of low thermal conductivity on the performance of seawater evaporation, the thermal efficiency ($\eta$) was calculated in term of the equation below:\textsuperscript{1, 7}:

$$\eta = \frac{Q_e}{Q_s} \quad (1)$$

where $Q_s$ is the total solar irradiation energy in three hours, and $Q_e$ is power consumed for seawater vapor generation in three hours, which can be estimated by the following equation,

$$Q_e = m \lambda + m C \Delta T$$

where $m$ is the mass of seawater vapor, $\lambda$ is the latent heat of the phase change, $C$ is the specific heat capacity of water ($4.2 \text{ J·g}^{-1}·\text{K}^{-1}$) and $\Delta T$ is the temperature increase of the water. The detailed data for seawater evaporation were shown in Table S2. Fe$_3$Si aerogel and bulk Fe$_3$Si supported on melamine foam showed an efficiency of 91.8 % and 70.7 % under the 1.0 kW·m$^{-2}$ of solar intensity.
Figure S9. Seawater evaporation performance of Fe$_3$Si aerogel/melamine foam under 1.0, 2.0 and 3.0 kw·m$^{-2}$ of sunlight irradiation (1 to 3 sun).
Figure S10. (a) The water contact angle of pristine Fe₃Si aerogel. A water droplet is loaded on the surface of a sample disc, which was prepared by pressing materials. (b) The picture of pristine Fe₃Si aerogel sink in water photographed by camera.
Figure S11. (a, b) The extra five-cycle water evaporation performances of hydrophobic Fe$_3$Si aerogel floated on 0.5 M H$_2$SO$_4$ and 1 M NaOH solutions, respectively, under 1.16 kw·m$^{-2}$ solar illumination. It is revealed that the water evaporation amounts of extra 5 cycles is gradually reduced from 4.05 to 3.55 Kg m$^{-2}$ in 0.5 M H$_2$SO$_4$ solution and 3.50 to 3.07 Kg m$^{-2}$ in 1 M NaOH solution, both of which were almost similar to the first five-cycles of water evaporation performance, revealing the excellent stability of hydrophobic Fe$_3$Si aerogel. The slight decrease of water evaporation rate during cycles test is possibly induced by the residual adsorption of H$_2$SO$_4$ and NaOH on Fe$_3$Si aerogel.
Figure S12. (a, b) SEM images of hydrophobic Fe$_3$Si aerogel after 10 cycles of photothermal water evaporation form 0.5 M H$_2$SO$_4$ and 1 M NaOH, respectively. The SEM images showed that hydrophobic Fe$_3$Si aerogel still maintained porous structure of pristine Fe$_3$Si aerogel, without any significant structure degradation. (c, d) Water contact angles of hydrophobic Fe$_3$Si aerogel after 10 cycles of photothermal water evaporation form 0.5 M H$_2$SO$_4$ (contact angel of 110°) and 1 M NaOH (100°), respectively. A water droplet is loaded on the surface of a sample disc prepared by pressing materials. In comparison with pristine hydrophobic Fe$_3$Si aerogel of 110°, it is suggested that Fe$_3$Si aerogel was more suitable for photothermal water evaporation from H$_2$SO$_4$. 
Figure S13. (a) SEM image of porous carbon. (b) and (c) Photographs of porous carbon loaded in 0.5 M H₂SO₄ and 1 M NaOH solutions under 1.16 kw·m⁻² of sunlight illumination for 1 day. It is clearly seen that, after 1 day, porous carbon was completely deposited at the bottom of H₂SO₄ and NaOH solutions, indicative of unapplicablity for the corrosive water evaporation.

Synthesis of porous carbon: 1 g of glucose was dissolved in 5 ml of H₂O, and subsequently added into 20 g of NaCl powder with agitation. After that, the mixture was treated by liquid nitrogen, freeze dried, and annealed in the tube furnace with N₂ atmosphere of 100 sccm at 1000 °C for 2 h. Porous carbon was obtained after washing the NaCl with deionized water three times.
Figure S14. (a) Water evaporation rate under dark circumstances and (b) the corresponding calculated equivalent enthalpy in different conditions of pure water, 0.5 M of H$_2$SO$_4$ solution, and hydrophobic Fe$_3$Si aerogel floated on H$_2$SO$_4$ solution. Note that the different water evaporation cells were put in same dark room at same time under a temperature of 18 °C, and the value of ΔH$_1$ was 2458 KJ·kg$^{-1}$ under 18 °C.
Calculation of Thermal Radiation Power

The heat loss of thermal radiation of Fe$_3$Si aerogel on seawater, 0.5 M H$_2$SO$_4$ and 1 M NaOH solution, respectively, was calculated based on Stefan-Boltzmann law:

\[ j = \varepsilon \sigma (T_2^4 - T_1^4). \]

Where \( j \) is the thermal radiation power, \( \sigma \) is the emissivity, and \( T \) is Kelvin temperature (K) of materials. The emissivity was 0.88 for Fe$_3$Si aerogel. For seawater, 0.5 M H$_2$SO$_4$ and 1 M NaOH solution, the ambient temperature was 23, 18, and 18 °C (296, 291, 291 K, \( T_1 \)), respectively, and the temperature of irradiated Fe$_3$Si aerogel was 52, 84, and 84 °C (325, 357, 357 K, \( T_2 \)), respectively. Therefore, the calculated values \( j \) are 0.08, 0.44 and 0.44 kW·m$^{-2}$ for seawater, 0.5 M H$_2$SO$_4$ and 1M NaOH solution, respectively.
References


