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Flatband λ-Ti_3O_5 boosts solar evaporation

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Interfacial solar evaporation is regarded as a promising strategy for water purification, and materials with high evaporation performance have been continually explored. Recently in *Nature*, Yang et al. reported that flatband λ-Ti_3O_5-integrated hydrogel-based evaporators achieve an ultrahigh water evaporation rate of 6.09 kg m^{-2} h^{-1} under 1 sun irradiation.

Freshwater resources are increasingly strained due to pollution, population growth, and climate change.[1] Interfacial solar evaporation is regarded as a sustainable strategy to alleviate the freshwater crisis.[2] For realizing efficient solar evaporation, a variety of photothermal materials have been developed and integrated into two-dimensional (2D) or three-dimensional (3D) evaporators, including metallic nanoparticles, carbon-based materials, narrow-bandgap semiconductors, and hybrid hydrogels.[2–5] Currently, continuous research efforts are being devoted to seeking out photothermal materials with better performance of solar energy harvesting and evaporation.

In a recent work published in *Nature*,[6] Professor Liang Zuo and his team propose a novel approach to elevate joint densities of states (JDOSs) for solar absorption enhancement by introducing a flatband electronic structure. Their study shows that flatband λ-Ti_3O_5 powders exhibit high solar absorptivity of 96.4%. When incorporated into 2D/3D evaporators, the Ti–Ti dimers and U-shaped groove structure on the λ-Ti_3O_5 surface promote the dissociation of adsorbed water molecules and boost water evaporation. It is reported that 3D λ-Ti_3O_5-incorporated polyvinyl alcohol (PVA) hydrogel achieves an ultrahigh water evaporation rate of 6.09 kg m^{-2} h^{-1} under 1 sun irradiation.

For photothermal materials, solar absorptivity mainly relies on the characteristics of its photoexcited electron transitions. To enhance the solar absorptivity of the photothermal materials, the authors emphasize the importance of elevating JDOSs, which has been less explored in the previous studies of interfacial solar evaporators. Titanium suboxides (TSOs, Ti_nO_{2n-1}) have attracted the attention, as the presence of intrinsic oxygen deficiency in TSOs provides opportunities for the formation of distinct Ti–Ti dimers with diverse electronic band structures. Combined theoretical and experimental studies on Ti_nO_{2n-1} ($n \leq 4$) reveal that all these TSOs demonstrate overall low reflectivities across the solar spectrum due to their common feature of relatively flat bands around the Fermi level (E_F). Such flat bands not only expand the spectrum for solar absorption but also generate high JDOSs for efficient optical transitions, resulting in a generally enhanced solar absorptivity.

Among the TSOs, the metallic λ-Ti_3O_5 stands out with the highest mean solar absorption of 96.4% as its low-lying bands exhibit almost no dispersion across the entire Brillouin zone, and both intraband and interband optical transitions can occur (Figures 1A–1C). Further computational tests show that if removing the low-lying flat band, the resultant solar absorptivity would be significantly reduced. These results confirm the authors' idea of improving solar absorptivity through the modulation of electronic band structures, specifically through Ti–Ti dimer-induced flat bands with high JDOSs.

In addition to the high solar absorption, it is also found that λ-Ti_3O_5 helps to boost

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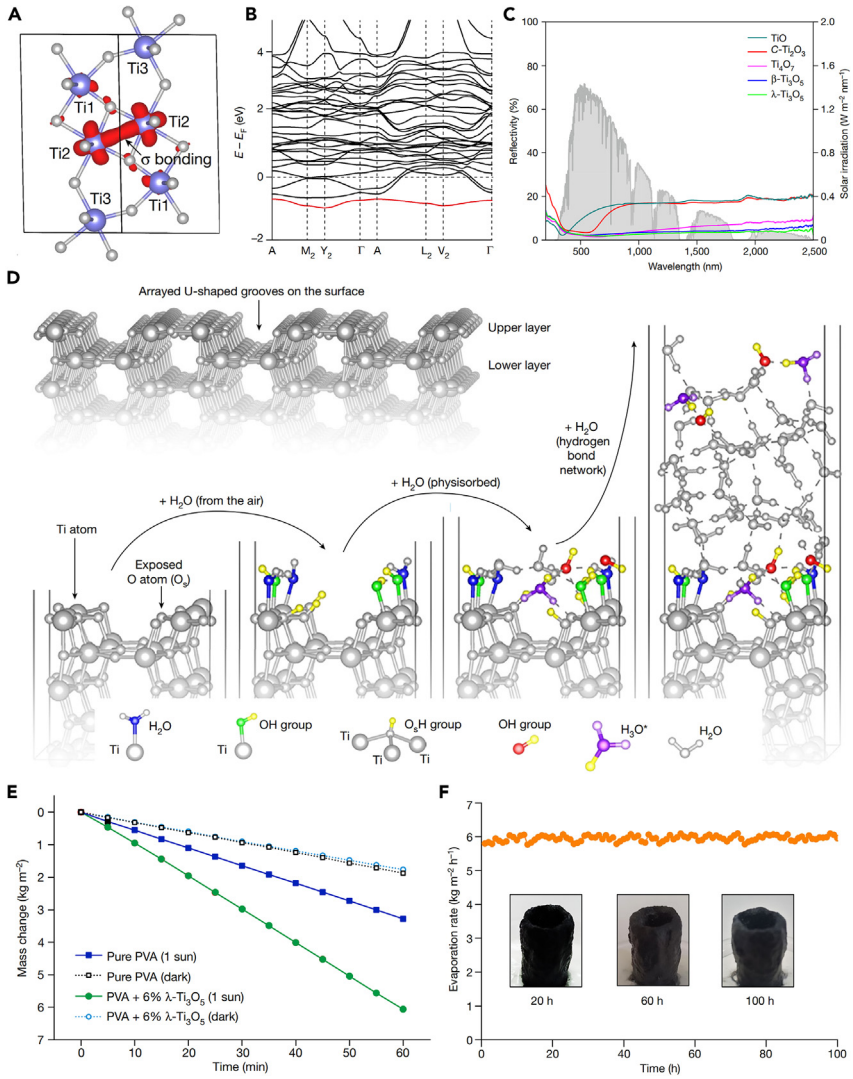

Figure 1. Flatband λ-Ti_3O_5 for boosting solar evaporation

(A) Isosurface of the calculated charge density with an isovalue of 0.1 e Å^{-3} for the low-lying flat band of λ-Ti_3O_5 to show the charge localization along with the Ti2–Ti2 dimer.

(B) Band structure of λ-Ti_3O_5.

(C) Reflectivity spectra of Ti_nO_{2n-1}, $n \leq 4$ (TiO, *C*-Ti_2O_3, λ-Ti_3O_5, β-Ti_3O_5, and Ti_4O_7), along with the frequency-dependent solar spectrum in gray background.

(D) Schematics of the λ-Ti_3O_5 (1 $\bar{1}$ 0) surface and water adsorption and dissociation on λ-Ti_3O_5 (1 $\bar{1}$ 0) surface.

(E) Mass changes of 3D evaporator containing λ-Ti_3O_5 powders under 1 sun illumination and dark conditions compared with pure PVA evaporator.

(F) Evaporation rates of 3.5 wt% saline water in 100 h for the 3D evaporator containing 6 wt% λ-Ti3O5 powders under 1 sun illumination. The insets show the photographs of the 3D evaporator at 20 h, 60 h, and 100 h without salt precipitation. Reprinted with permission from Yang et al.[6] Copyright 2023, Nature Publishing Group.

the evaporation rate. The λ-Ti_3O_5 incorporated 2D solar evaporator demonstrates a net dark-excluded evaporation rate of 1.42 kg m^{-2} h^{-1}, close to the theoretical limit (1.47 kg m^{-2} h^{-1}) of bulk water under 1 sun of irradiation. The high evaporation rate of the 2D evaporator is attributed to the reduced vaporization enthalpy of water on the surfaces of λ-Ti_3O_5 powders, which is estimated to be 1,696 kJ kg^{-1} by using the thermometric method, two-thirds of that of bulk water. The authors deem that both Ti–Ti dimers and exposed U-shaped grooves on the λ-Ti_3O_5 surface significantly contribute to water adsorption and dissociation, and the frequent occurrence of metastable H_3O^* units, coupled with rapid proton transfer, boosting the interfacial water evaporation through small clusters (Figure 1D). As the λ-Ti_3O_5 powders are dispersed into 3D porous hydrogel-based evaporators, they can realize an ultrahigh evaporation rate of 6.09 kg m^{-2} h^{-1} under 1 sun irradiation (Figure 1E). The 3D evaporator maintains the high evaporation rate without salt precipitation over 100 h when treating 3.5 wt % saline water (Figure 1F), offering an inspiring approach to realizing efficient solar desalination.

Reducing enthalpy to boost solar evaporation rate recently has aroused extensive research interest. Indeed, many researchers have observed evaporation rates exceeding the theoretical limit (1.47 kg m^{-2} h^{-1} under 1 sun illumination, assuming all solar energy is converted into heat and used for water evaporation) in different types of materials, from PVA to other polymers and even inorganic porous absorbers.[7] Some researchers attributed this to the reduction of vaporization enthalpy due to water evaporation through clusters.[7] However, providing rational explanations and relevant evidence remains a challenging task. It is inspiring that the authors offer a novel thought of the interaction between water and evaporator surface (λ-Ti_3O_5) for the reduction of vaporization enthalpy and formation of clusters. As the conclusions so far mainly rely on the simulation results, it calls for more experimental exploration. In a recent study, Professor Gang Chen and his group proposed a hypothesis of photomolecular effect for the trials of explaining the generation of water clusters and reported a series of experimental observations.[8] They believe that photons can cleave off water clusters from the surface region, which may explain many past

observations of the exceeding thermal limit evaporation under solar illumination. At present, it seems that there is no unified conclusion on the explanation of water clusters, and it calls for further research by the community.

In addition, the quality of the purified water needs attention when water evaporates in the form of clusters. It is reported that the Li^+ ions would be carried to the condenser during solar evaporation if the water evaporation proceeds in the form of clusters. Results show that the concentration of Li^+ ions in the condensed water by using the λ-Ti_3O_5-based evaporator is an order of magnitude higher than that without using the λ-Ti_3O_5-based evaporator when evaporating a water solution with the concentration of 100 g L^{-1} LiCl. While the results demonstrate that water may evaporate in the form of small clusters, it also shows that water clusters may carry salt ions during the evaporation process. This may lead to uncertainty of the quality of the purified water, especially when treating wastewater containing small-sized ions.

Constructing 3D evaporators is another effective approach for enhancing the evaporation rate, as 3D evaporators achieve a remarkable increment of evaporation rate by harnessing environmental energy for the evaporation. Evaporation rates over 10 kg m^{-2} h^{-1} under 1 sun illumination have been reported in the previous studies.[9] However, it is often challenging to maintain the high evaporation rate when scaling up toward practical applications due to the inevitable interference between the adjacent evaporation. It seems that evaporation enhancement achieved by reducing vaporization enthalpy can be maintained in principle when scaling up the evaporators. Thus, the contribution of reduced evaporation enthalpy to accelerated evaporation rate is worthy of being quantified and discussed in 3D materials. It is hoped that high solar evaporation rates over large areas can be achieved for practical applications in the future.

Currently reported high evaporation performances of solar evaporation technology have sparked considerable interest in applying it to various practical applications, including clean water production, wastewater treatment, resource recovery, sterilization, and so on.[10] Therefore, in addition to pursuing high evaporation rate, a different matrix of factors also needs to be taken into consideration to unleash full potential of solar evaporation for these applications (including water, energy, and medical), such as collected water flux for solar desalination, vapor mass flux for wastewater treatment, and recovery rate and purity for the resource recovery. It is hoped that with ongoing research efforts and deep global collaborations in the coming decades, our community will transform the solar evaporation technology toward viable industrialized/commercialized techniques.

DECLARATION OF INTERESTS

The authors declare no competing interests.

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