

# MoSi solar container transformation

How is a supercell model built in MoSi<sub>2</sub>N<sub>4</sub>?

As the substrate material, the calculated supercell model is built by 3×3×1 unit cell of MoSi<sub>2</sub>N<sub>4</sub> to avoid the interaction between the active sites from nearby models. The N atom on the MoSi<sub>2</sub>N<sub>4</sub> surface is replaced in sequence by 3 d and 4 d periods of TMSAs (i.e., Sc, Fe, Ni, Cu, etc.).

What is the power conversion efficiency of Type-II MoSi<sub>2</sub>?

Beyond 22% power conversion efficiency in type-II MoSi<sub>2</sub>As<sub>4</sub>/MoGe<sub>2</sub>N<sub>4</sub> photovoltaic vdW heterostructure +

How do photo-generated electrons transfer from MoSi<sub>2</sub> to MOGE<sub>2</sub>N<sub>4</sub>?

Computational assessments demonstrate that photo-generated electrons efficiently transfer from the MoSi<sub>2</sub>As<sub>4</sub> to the MoGe<sub>2</sub>N<sub>4</sub> layer, while holes move in the opposite direction, reducing electron-hole recombination.

Is MoSi<sub>2</sub>/Moge<sub>2</sub>n<sub>4</sub> a promising candidate for solar cell applications?

These results position the MoSi<sub>2</sub>As<sub>4</sub>/MoGe<sub>2</sub>N<sub>4</sub> heterostructure as a promising candidate for solar cell applications due to its superior optoelectronic properties.

Does MoSi<sub>2</sub>n<sub>4</sub> have a CO<sub>2</sub> RR photocatalytic performance?

Conclusions In summary, the CO<sub>2</sub> RR photocatalytic performances of MoSi<sub>2</sub>N<sub>4</sub> decorated with 3 d and 4 d TMSAs have been theoretically evaluated via DFT computations. Five single-carbon molecules (CO, HCOOH, HCHO, CH<sub>3</sub>OH, and CH<sub>4</sub>) are considered potential CO<sub>2</sub> RR products.

Is MoSi<sub>2</sub>n<sub>4</sub> a good photocatalyst?

Moreover, the MoSi<sub>2</sub>N<sub>4</sub> monolayer has also been shown to have good piezoelectric properties, high optical transmittance, high carrier mobility, and low electron-hole recombination rate. Excellent photo-response ability provides broad prospects for the application of CO<sub>2</sub> RR photocatalysts.

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By performing first-principles calculations, we systematically explore MoSi<sub>2</sub>N<sub>4</sub> decorated with 3 d and 4 d period transition metal single atoms (TMSAs) as efficient CO<sub>2</sub> reduction ...

The solar container is lifted using the corner corners in the roof frame. With these in the base frame, the



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module can be fixed and secured during transport using the twist-lock system.

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