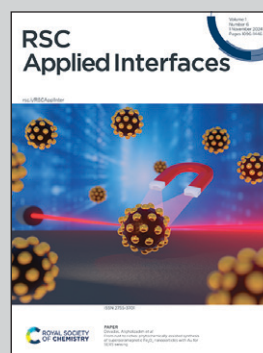


Showcasing research from Assistant Professor Yee Sin Ang's research group, Science Mathematics and Technology Cluster (SMT), Singapore University of Technology and Design (SUTD), Singapore.

Electric field and strain tunable band gap and band alignments of $\text{MoSi}_2\text{N}_4/\text{MSe}$ ($\text{M} = \text{In}, \text{Ga}$) van der Waals heterostructures

Using density functional theory simulations, it is demonstrated that $\text{MoSi}_2\text{N}_4/\text{MSe}$ ($\text{M} = \text{In}, \text{Ga}$) van der Waals heterostructures host highly tunable electronic properties. Their band structures can be tuned between Type-I and Type-II alignment, thus suggesting the potential of $\text{MoSi}_2\text{N}_4/\text{MSe}$ heterostructures for a large variety of applications such as solar cell, photodetector and light-emitting diodes. These findings shed light on the capability of MoSi_2N_4 -based heterostructures for electronics and optoelectronics device applications.

As featured in:



See Yee Sin Ang, L. K. Ang *et al.*, *RSC Appl. Interfaces*, 2024, 1, 1156.