

Abstract Submitted
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Computational Design of 2D materials for Energy Applications

QIANG SUN, Peking University — Since the successful synthesis of graphene, tremendous efforts have been devoted to two-dimensional monolayers such as boron nitride (BN), silicene and MoS₂. These 2D materials exhibit a large variety of physical and chemical properties with unprecedented applications. Here we report our recent studies of computational design of 2D materials for fuel cell applications which include hydrogen storage, CO₂ capture, CO conversion and O₂ reduction.

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