Opportunities and challenges for 2D heterostructures in battery applications: a computational perspective

Abstract

With an increasing demand for large-scale energy storage systems, there is a need for novel electrode materials to store energy in batteries efficiently. 2D materials are promising as electrode materials for battery applications. Despite their excellent properties, none of the available single-phase 2D materials offers a combination of properties required for maximizing energy density, power density, and cycle life. This article discusses how stacking distinct 2D materials into a 2D heterostructure may open up new possibilities for battery electrodes, combining favourable characteristics and overcoming the drawbacks of constituent 2D layers. Computational studies are crucial to advancing this field rapidly with first-principles simulations of various 2D heterostructures forming the basis for such investigations that offer insights into processes that are hard to determine otherwise. We present a perspective on the current methodology, along with a review of the known 2D heterostructures as anodes and their potential for Li and Na-ion battery applications. 2D heterostructures showcase excellent tunability with different compositions. However, each of them has distinct properties, with its own set of challenges and opportunities for application in batteries. We highlight the current status and prospects to stimulate research into designing new 2D heterostructures for battery applications.