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Assessing the Suitability of α-SiS Nanosheet as an Anode Material for Multivalent Metal-Ion Batteries

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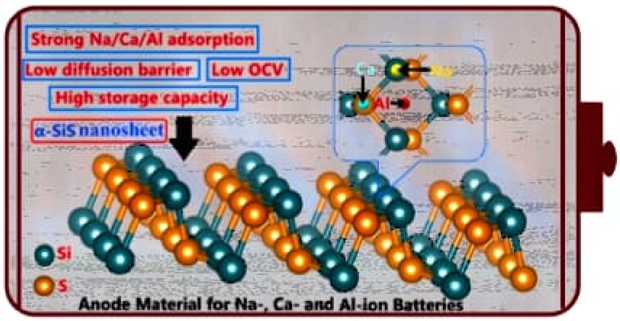

ABSTRACT: The search for suitable two-dimensional (2D) anode materials is crucial to drive the progress of multivalent metal-ion batteries capable of delivering exceptional performance, specifically with very fast charging and discharging rates. In this research, we have unveiled novel insights at the density functional theory level, with the workability of 2D puckered silicon monosulfide (α-SiS) as a probable anode material for multivalent metal-ion batteries using Na, Ca, and Al ions. Exploring the stability aspects of both structural and dynamic levels in the α-SiS nanosheet was estimated through the calculation of cohesive energy and non-imaginary phonon frequencies. The α-SiS nanosheet exhibited negative adsorption energies of −1.45, −0.92, and −2.67 eV for Na, Ca, and Al ions, respectively. Additionally, it was observed that the introduction of mono-, di-, and tri-metal atoms to the surface of the α-SiS nanosheet transformed its semiconducting nature into a metallic phase. Minimal activation energies for the active ion migration of Na (0.066 eV), Ca (0.067 eV), and Al (0.18 eV) on the surface of the α-SiS nanosheet suggest high diffusion and optimal charge/discharge functionality. Furthermore, diminished mean operating voltages of 0.44 V (Na), 0.43 V (Ca), and 0.55 V (Al) were attained and improved the theoretical storage performance of 2046.81 mAh/g (Na), 1643.02 mAh/g (Ca), and 2422.76 mAh/g (Al) for the α-SiS nanosheet. The results of this work suggest that the α-SiS nanosheet has the potential to play a crucial role as a hopeful anode material for the creation of budget-friendly, high-functioning metal-ion batteries using Na, Ca, and Al ions.

■ INTRODUCTION

Our energy policy is still largely focused on the use of non-sustainable fuel sources, which are leading drivers of CO_2-induced global climate disruption. A survey in 2018 found that 89% of worldwide CO_2 expulsions originated from industry and traditional energy sources, with coal being the dirtiest conventional fuel and responsible for more than 0.3 °C of the 1 °C climatic temperature elevation. Therefore, it is the chief contributor to Earth's climatic temperature upsurge. On the other hand, burning oil is responsible for around one-third of global carbon emissions, while natural gas is typically marketed as a more environmentally friendly green energy resource in comparison to coal and oil but is also responsible for one-fifth of global carbon emissions.[1,2] In view of these environmental concerns and the limitations associated with energy security issues of non-renewable fossil fuels, efforts are being made to optimal utilization of sustainable energy resources. However, renewable energy sources are unpredictable as a result of their reliance on atmospheric conditions, region, productivity, and established framework; therefore, effective grid-scale energy storage units are needed to store, transport, and use the energy generated by these sources. To address this need, low-cost electrical energy storage devices, such as rechargeable batteries, which have been a key enabler of the smart grid or future grid, are expected to play a significant role in incorporating a large proportion of renewable energy while also providing electricity for hybrid and electric vehicles.[3−6] Among the various types of low-cost electrical energy storage devices, alkali metal-ion batteries, such as lithium-ion batteries, are particularly popular by virtue of their high energy and power density.[7] However, even though lithium-ion batteries have high energy density and extended durability, the finite lithium reserves in the Earth's crust and the resulting high cost of the batteries limit their future development.[8−11] These issues highlight the need for

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