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Title: First-Principle Study of the Electronic Structure of Low Dimensional Materials and Their Related Applications

We introduce the background in the relevant fields including the introduction of two-dimensional layered materials (2DLMs) and their applications in first chapter. Density functional theory is described in second chapter.

In chapter three, we discuss the adsorption properties of molecules NH_3, CH_4 and H_2O on pristine and indium doped phosphorene (In@P). We systematically investigate structural, electronic and transport properties of In@P along with pristine phosphorene (PP). We found that all three molecules are physisorbed on In@P, and NH_3 and H_2O can be detected with high sensitivity.

In chapter four, we explore the structural, mechanical and diffusion properties of Ga_{100} with and without Na-atom. It is established that the Ga_{100} ML is one of the promising anode materials for Na-ion batteries.Our diffusion calculations conclude that the Ga_{100} ML can possess a high charge/discharge rate with a diffusion barrier of 0.36 eV for Na-ion batteries. The theoretical storage capacity of 961.30 mAh/g is found. The average open-circuit voltage of 0.52 eV for Na adsorption is found. In conclusion, our findings guide toward the possibility of using the Ga_{100} ML for Na-ion battery anodes.

To further improve the performance of energy storage devices, in chapter five, we present the 2D van der Waal heterostructure constructed from Blue phosphorene and C_3N monlayer for the alkali metal-ion batteries. We reported that the energy barrier (0.046 eV) for Na ions is the lowest among the three for the various diffusion pathways. Furthermore, the HS also possesses a large storage capacity (1511.44 $mAhg^{-1}$) for Na. Based on our findings, we believe that the C_3N/BP HS could be used as a potential anode material for Li, Na and K-ion batteries.

Finally in the last chapter six, the conclusion and the future scope of the research work have been discussed.