First Principle Study of New W₂N Monolayer: a Promising Candidate for Li⁺ ion Batteries

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We have predicted new anode material W₂N monolayer for the application of Li⁺ ion batteries by using first principles calculation. The W₂N monolayer is found to be stable energetically and dynamically as well. It is also found that W₂N monolayer is metallic in both IT phase and in 2H phase. Furthermore, the calculated open circuit voltage for the Li⁺ adsorbed W₂N monolayer is 0.88V which is suitable voltage for a commercial anode material. The calculated diffusion barrier for the Li⁺ ions on the surface of W₂N monolayer is 0.22eV. Due to low diffusion barrier the ions will easily flow over the surface of W₂N monolayer. This will boost the electronic conductivity which is the requirement of an efficient Li⁺ ion battery.

Keywords: W₂N monolayer, electronic structure, Li⁺ ion battery, adsorption and binding energy, storage capacity, open circuit voltage.

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