Regular paper

A Novel Phase Parameter Estimation Method of Quadratic FM Signal based on Sigmoid Fractional Ambiguity Function in Impulsive Noise Environment

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First-Principles Study of monolayer $SnS_{2(1-x)}Se_{2x}$ alloys as anode materials for Lithium ion Batteries

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Abstract: Based on density functional theory, the performance of the monolayer $SnS_{2(1-x)}Se_{2x}$ alloys with variation of x = 0, 0.25, 0.5, 0.75, 1 as the anode material for using in Lithium-ion batteries (LIBs) are examined. Numerical results show that the values of the band gap of $SnS_{2(1-x)}Se_{2x}$ alloys decrease with the increase of Se concentration. For Li adsorption, the alloys changed from semiconductor to metal after the insertion of Li and becomes suitable for being used as electrode material. Also, the low barrier energy is kept and the adsorption strength is enhanced in the $SnS_{2(1-x)}Se_{2x}$ alloys compared with that of the pristine SnS_2 system. With increased concentration of Se, little influence on the average open circuit voltage (OCV) value is observed, though the capacity of the system decreases from 293 to 194 mAh/g.

Keywords: Lithium ion Batteries; $SnS_{2(1-x)}Se_{2x}$ alloy; First-principle calculation

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