Rational designation of P-based compounds with fast diffusion ability as an anode material for sodium-ion batteries

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Sodium-ion batteries (SIBs) are receiving increasing interesting today because they are viewed as ideal candidates that can at least partially substitute for Li-ion batteries.[1, 2] The anode materials are important components of SIBs, but exploiting anode materials with fast kinetics is still a big challenge.[3, 4] Using first-principles calculations, rationally predicted electronic conductivity, ionic conductivity, and phase separation behaviors in a GeP_3 compound compared to those properties in black phosphorus (BP) are expected to lead to high-power-density anodes for SIBs. Considering elastically softened structures, calculated Na^+ migration barriers in sodiated GeP_3 structure are lower than those in sodiated BP structure (Figure 1a), identified by higher Na^+ diffusion coefficients obtained from GITT measurements of a GeP_3 electrode. On the basis of thermodynamic phase stabilities determined by mixing enthalpy values, phase filed simulations coupled with homogeneous bulk free energies for phenomenological descriptions predict that a phase separation reaction do not occur in BP. However, the suppressed phase separation behaviors of GeP_3 are confirmed by homogeneous Na^+ distributions using TEM EDS color mappings. The GeP_3 electrode delivers high capacities of 1.226, 1.061, 0.924, 0.790, and 0.578 Ah g^{-1} at 0.2, 0.5, 1, 2, and 5 A g^{-1}, respectively (Figure 1b). Even at an ultrahigh current density of 20 A g^{-1}, the capacity of GeP_3 electrode still maintains 0.197 Ah g^{-1}. At 1 A g^{-1}, the GeP_3 could maintain a discharge capacity of 0.499 Ah g^{-1} after 1000 cycles. Taking into account the three enhanced properties, the GeP_3 electrode presents a superior rate capability as compared with the BP electrode.

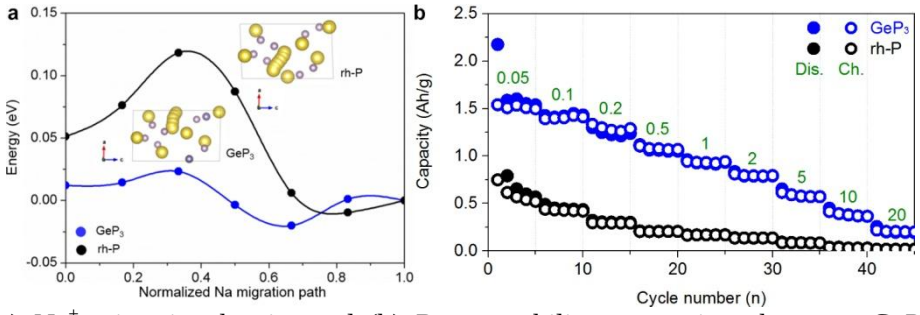

Figure 1. (a) Na^+ migration barrier and (b) Rate-capability comparison between GeP_3 and black phosphorus (BP).

References:

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