Supporting Information

High-Performance Lithium-Selenium Batteries Promoted by Heteroatom-Doped Microporous Carbon

Ziqi Yi, Lixia Yuan*, Dan Sun, Zhen Li, Chao Wu, Wenjuan Yang, Yanwei Wen, Bin Shan* and Yunhui Huang*

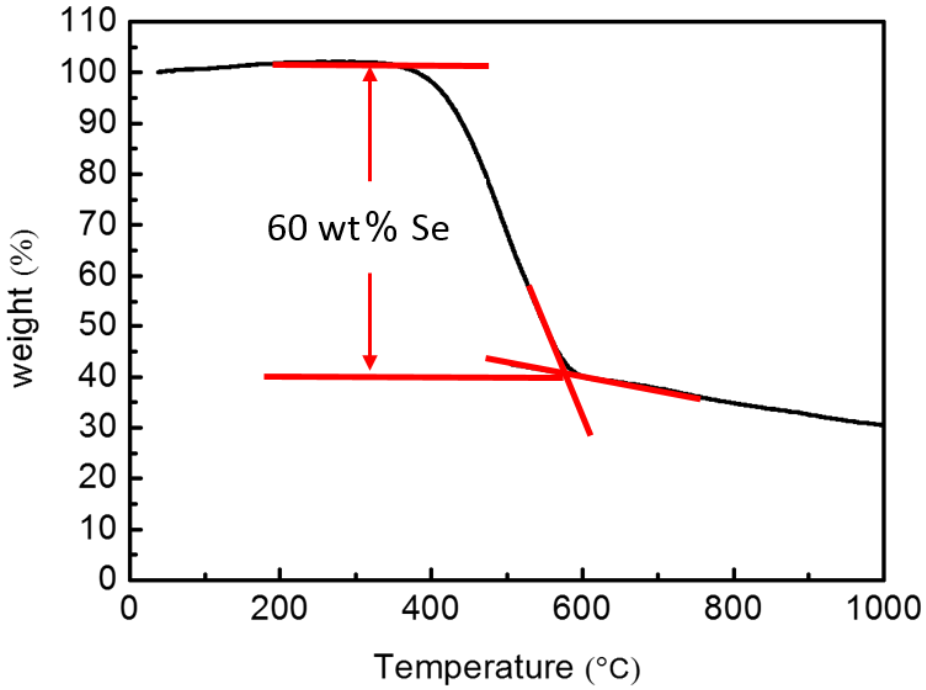

Figure S1 (TGA) curve of the Se-CP composite.

Details of first principle calculation

Our calculations are based on the density functional theory (DFT) with the Perdew–Burke–Ernzerh of version of the generalized gradient approximation (GGA-PBE)[1] for the exchange-correlation potential, as implemented in a plane-wave basis code VASP,[2,3] The pseudo-potential is described by the projector-augmented-wave (PAW)[4] method. An energy cutoff of 400 eV and 1×1×1 k-point with a Γ centered k mesh are used in our calculations. The atomic coordinates are fully relaxed using the conjugate gradient method[1] until the force on each atom is converged to less than 0.02 eV/Å.

References

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