Supporting Information

High Ion Mobility and Capacity of Monolayer GaS as a Promising Anode Battery Material

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Figure S1: Top and side view of atomic structure of $M_{0.031}\text{GaS}$ (a), $M_{0.056}\text{GaS}$ (b), $M_{0.125}\text{GaS}$ (c), and $M_{0.5}\text{GaS}$ (d) ($M = \text{Li, Na, K, Al}$).
**Figure S2:** Top and side view of atomic structure of Li$_1$GaS (a), Li$_{1.5}$GaS (b), Li$_2$GaS (c), and Li$_{2.5}$GaS (d).

**Figure S3:** ELF map of the (100) face of ML Li$_2$GaS (a), Li$_{2.5}$GaS (b).
Figure S4: ELF map of the (100) face of ML Na$_{0.125}$GaS (a), Na$_{0.5}$GaS (b).

Figure S5: ELF map of the (100) face of ML K$_{0.125}$GaS (a), K$_{0.5}$GaS (b) and K$_{1}$GaS (c).

Figure S6: ELF map of the (100) face of ML Al$_{0.125}$GaS (a), Al$_{0.5}$GaS (b).