

Supporting Information

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

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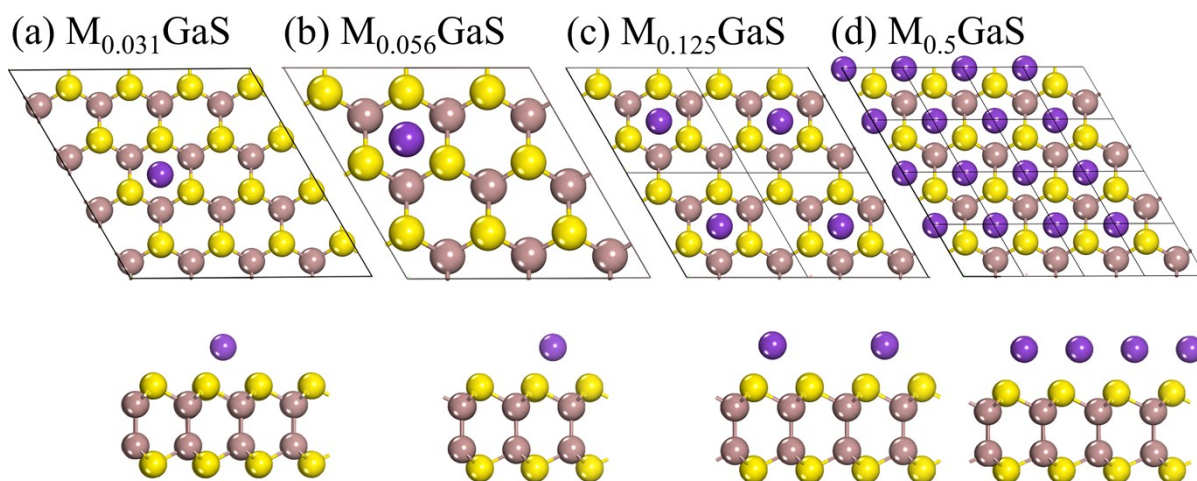


Figure S1: Top and side view of atomic structure of $M_{0.031}\text{GaS}$ (a), $M_{0.056}\text{GaS}$ (b), $M_{0.125}\text{GaS}$ (c), and $M_{0.5}\text{GaS}$ (d) ($M = \text{Li, Na, K, Al}$).

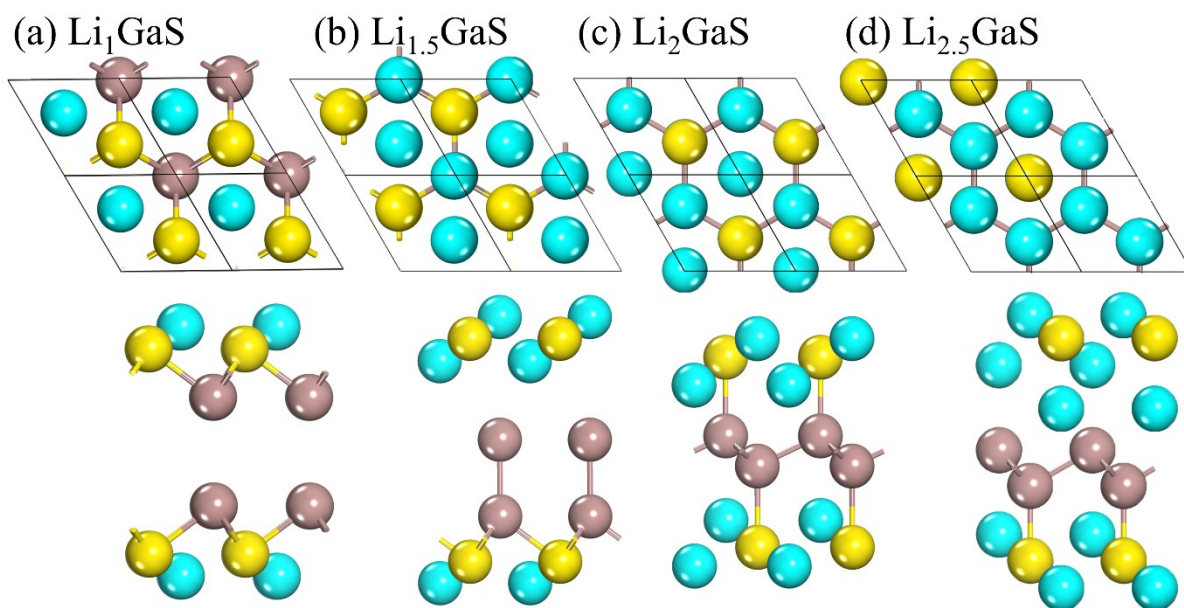


Figure S2: Top and side view of atomic structure of Li_1GaS (a), $\text{Li}_{1.5}\text{GaS}$ (b), Li_2GaS (c), and $\text{Li}_{2.5}\text{GaS}$ (d).

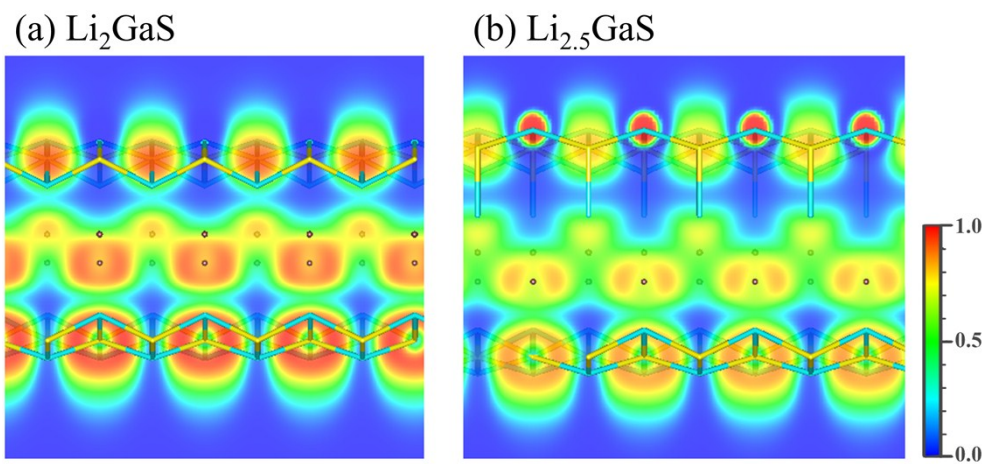


Figure S3: ELF map of the (100) face of ML Li_2GaS (a), $\text{Li}_{2.5}\text{GaS}$ (b).

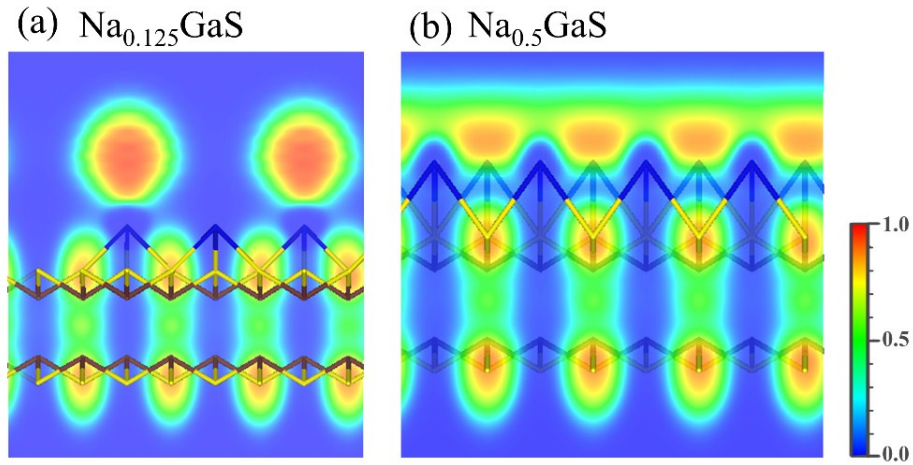


Figure S4: ELF map of the (100) face of ML $\text{Na}_{0.125}\text{GaS}$ (a), $\text{Na}_{0.5}\text{GaS}$ (b).

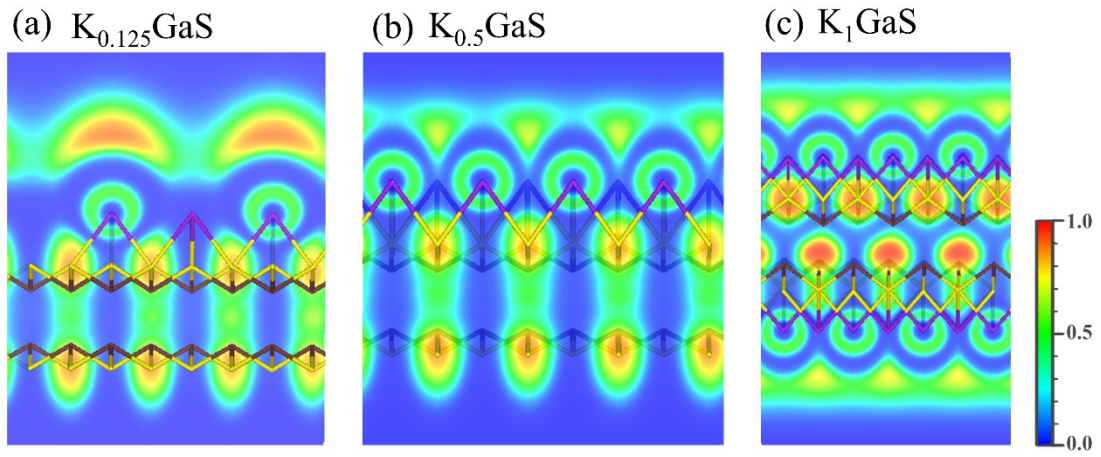


Figure S5: ELF map of the (100) face of ML $\text{K}_{0.125}\text{GaS}$ (a), $\text{K}_{0.5}\text{GaS}$ (b) and K_1GaS (c).

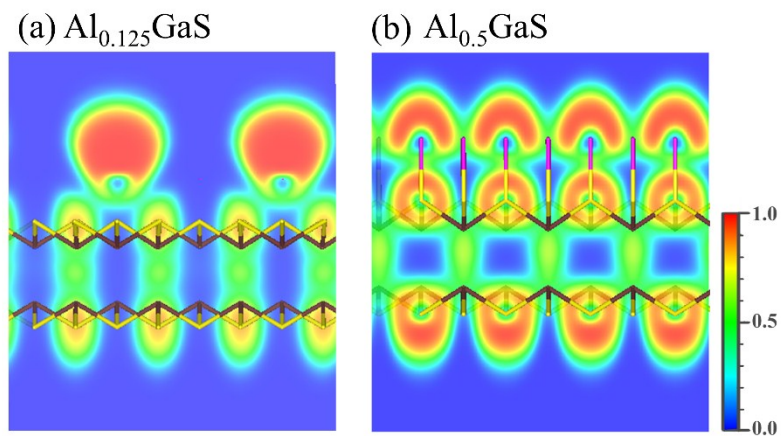


Figure S6: ELF map of the (100) face of ML $\text{Al}_{0.125}\text{GaS}$ (a), $\text{Al}_{0.5}\text{GaS}$ (b).