Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information for

Theoretical Prediction and Characterization of Novel Two-Dimensional Ternary Tetradymite Compounds La_2X_2Y (X = I, Br, Cl; Y = Ge, Te) as Anode Materials for Metal-Ion Batteries

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Supporting figures:

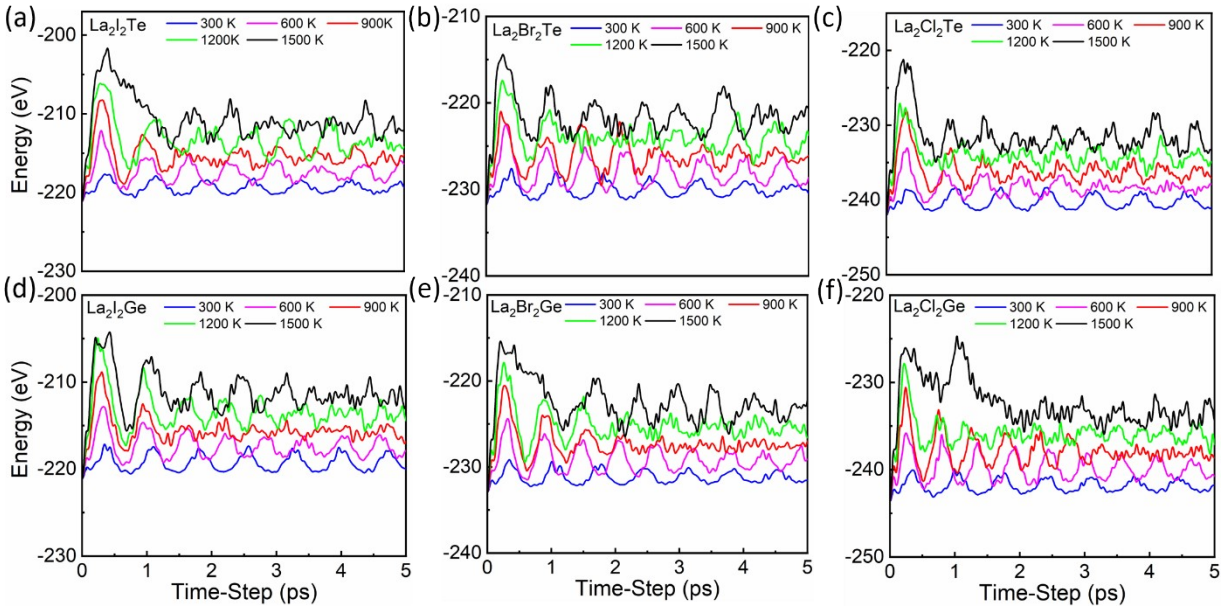

Fig. S1 Evolutions of the total energy of La_2X_2Y (X = I, Br, Cl; Y = Ge, Te) nanosheets during the AIMD simulations from 300-1500 K up to 5 ps. These results indicate that La_2X_2Y nanosheets are thermodynamically stable.

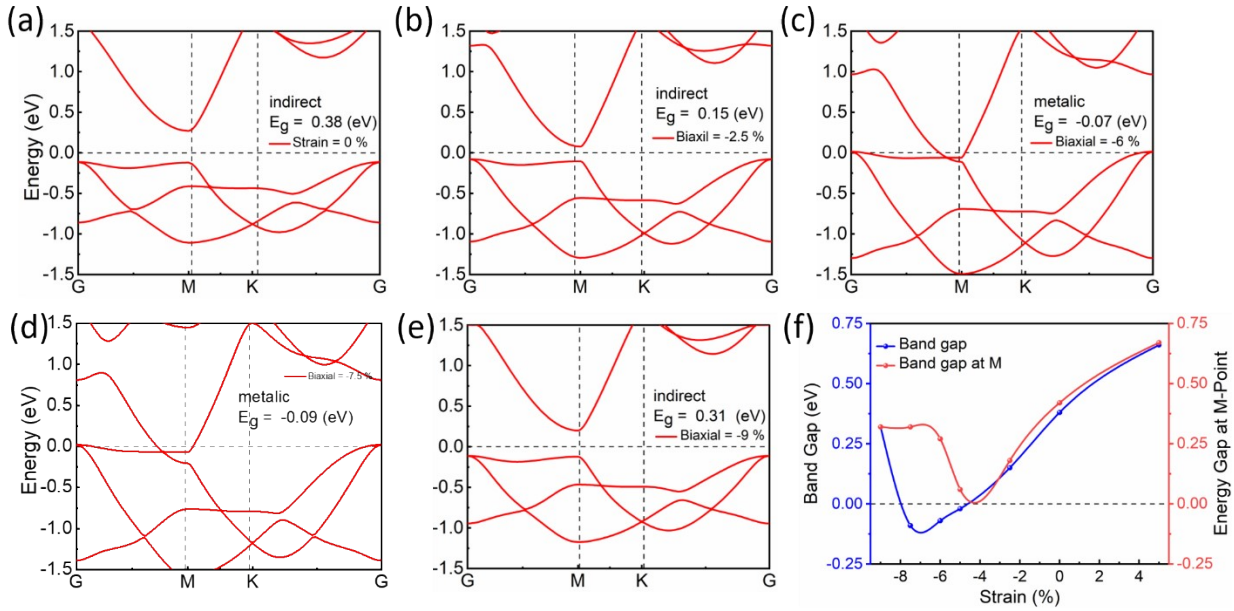

Fig. S2 Electron band structure of La_2I_2Ge, (a) no strain (b), 2.5% (c), 6 % (d) 7 % (e) 9 % biaxial compressive strain. And (f) depicts that band gap nearly closes at 6 % compressive strain, and reopens with further increase of the compressive strain.

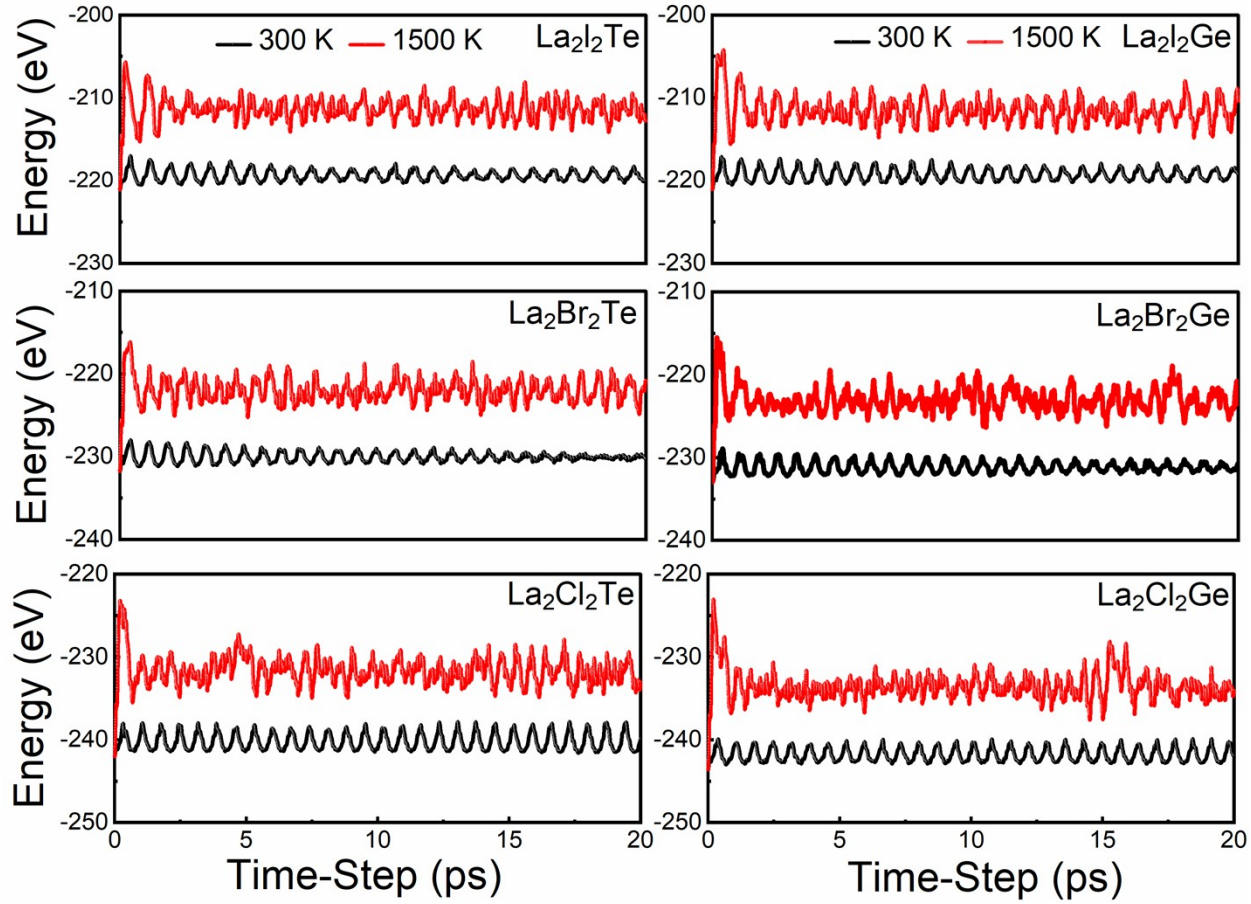

Fig. S3 Evolutions of the total energy of La_2X_2Y (X = I, Br, Cl; Y = Ge, Te) nanosheets during the AIMD simulations at 300, and 1500 K up to 20 ps. These results indicate that La_2X_2Y nanosheets are thermodynamically stable.

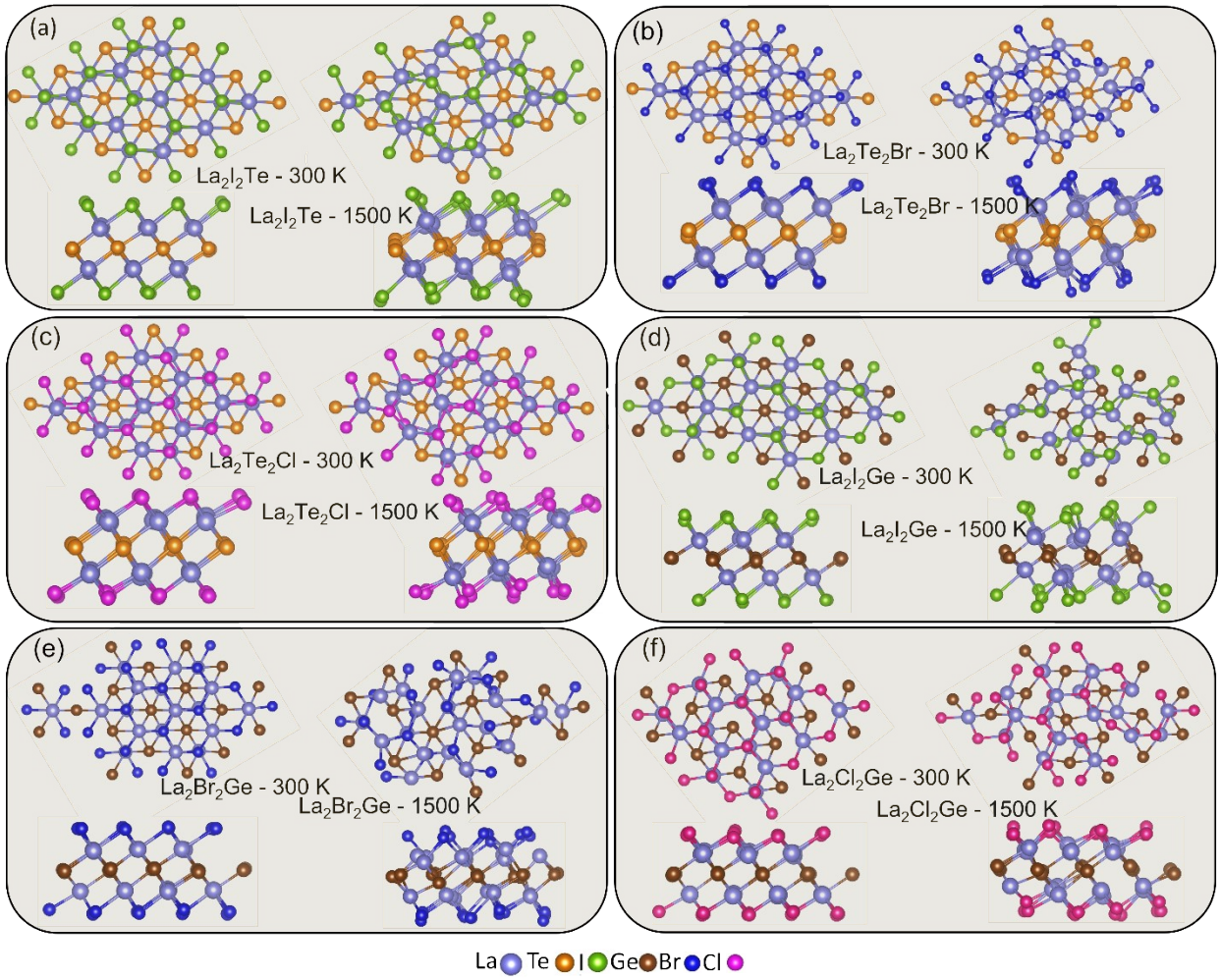

Fig. S4 Geometric structure of La_2X_2Y (X = I, Br, Cl; Y = Ge, Te) nanosheets during the AIMD simulations at 300, and 1500 K, simulated up to 20 ps. Geometrics structure indicate that La_2X_2Y nanosheets are thermodynamically stable.

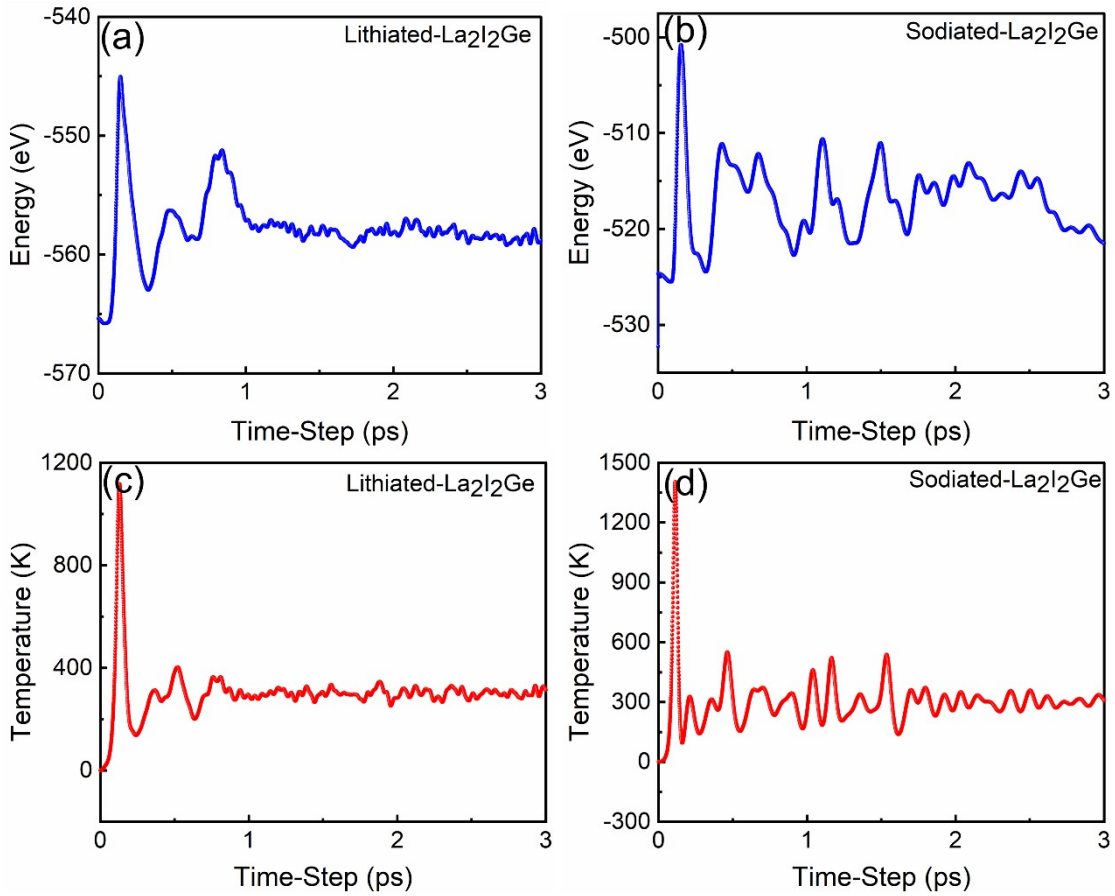

Fig. S5 Evolutions of the total energy and temperature of fully lithated and sodiated La_2I_2Ge nanosheets during the AIMD simulations at 300 up to 3 ps. These results indicate that La_2I_2Ge nanosheets are thermodynamically stable.

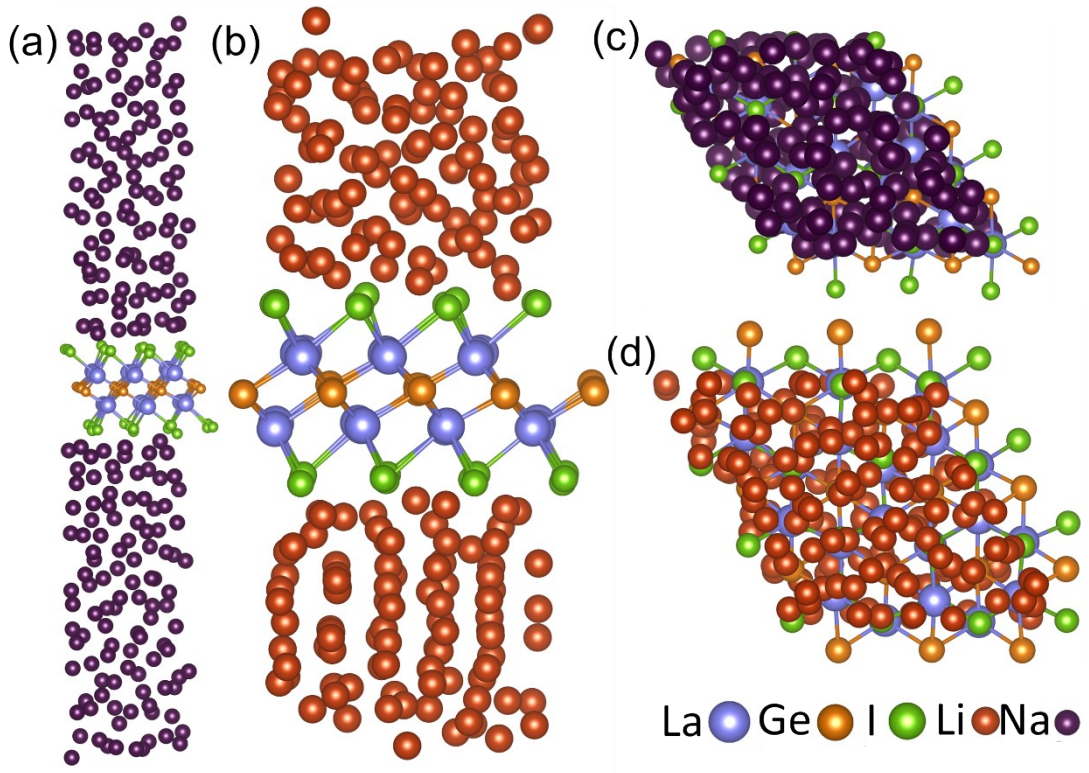

Fig. S6 Geometric configurations of La_2I_2Ge nanosheets during AIMD simulations at 300K over 3 ps. (a, b) Side views; (c, d) Top views. The structures suggest thermodynamic stability in fully lithiated/sodiated states.

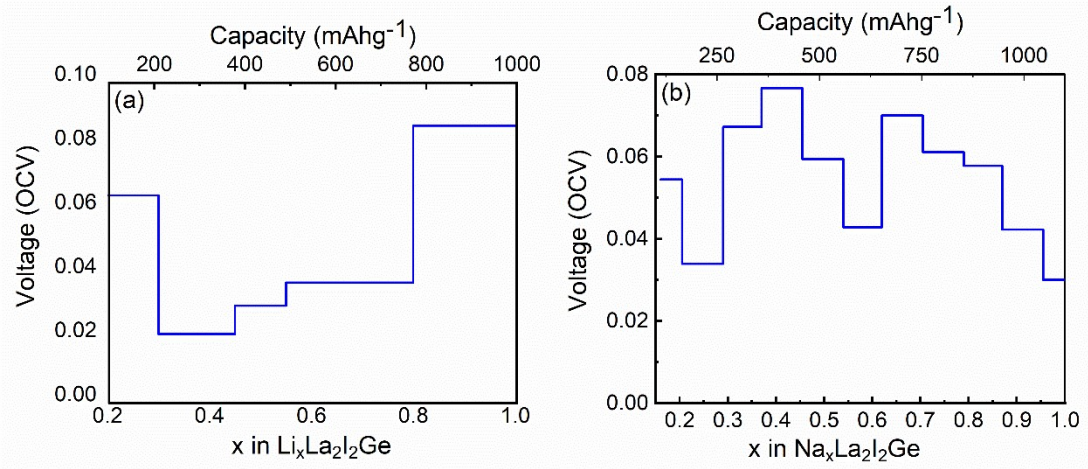

Fig. S7 Open-circuit voltage (OCV) as a function of the (a) Li concentration x, and (b) Na concentration x