Erratum: Data-Driven Prediction of Thermal Conductivity from Short MD Trajectories: A GCN-LSTM Approach [Chin. Phys. Lett. 43 020801 (2026)]

Shihao Feng[1,2], Haifeng Chen[1], Jian Zhang[2], Meng An[2*], and Gang Zhang[2*]

[1] *College of Mechanical and Electrical Engineering, Shaanxi University of Science and Technology, Xi'an 710049, China*

[2] *Yangtze Delta Region Academy in Jiaxing, Beijing Institute of Technology, Jiaxing 314019, China*

(Received 3 March 2026; accepted manuscript online 4 March 2026)

DOI: 10.1088/0256-307X/43/3/030804 CSTR: 32039.14.0256-307X.43.3.030804

In our recently published paper,[1] a typesetting error occurred during the production process. Figure 1 in the published version was incomplete. The processing of molecular dynamics (MD) simulation data into graph-structured representations in the left bottom panel of the figure was inadvertently omitted.

The complete and correct version of Fig. 1 is provided below. The figure caption remains unchanged.

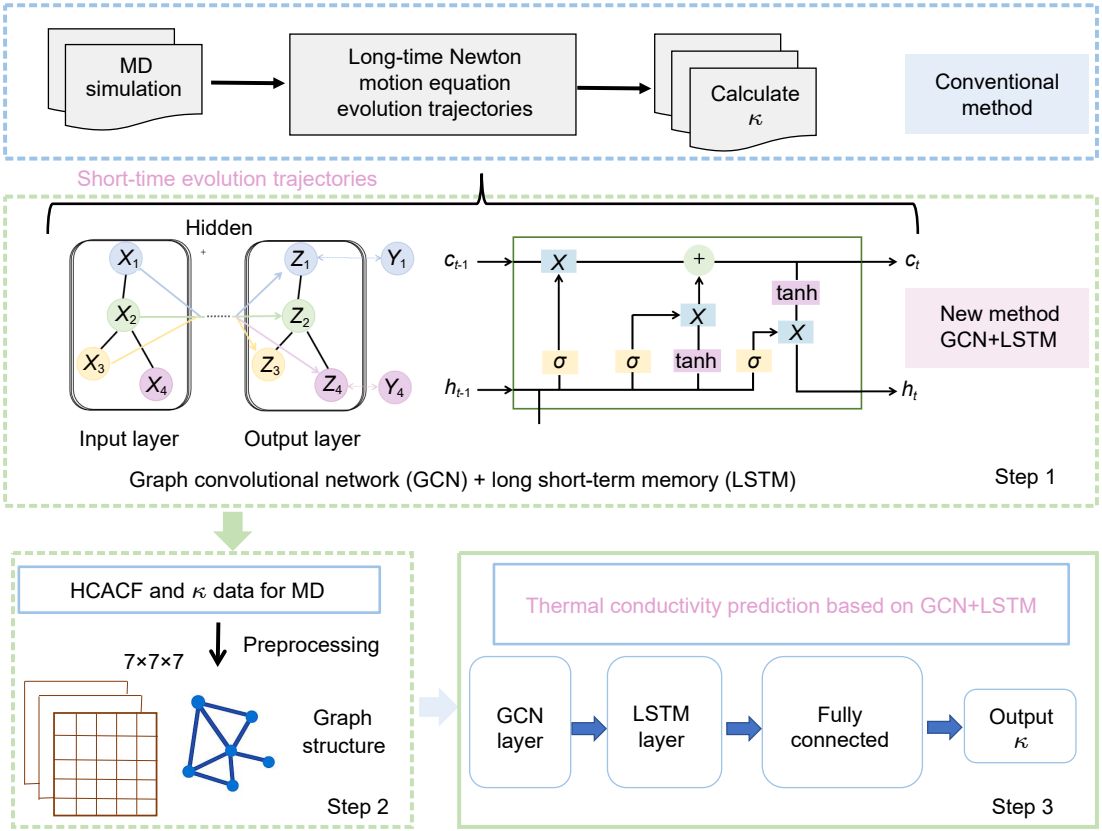

Fig. 1. Schematic overview of the ML-accelerated molecular simulation framework for thermal conductivity prediction. Starting from initial atomic configuration structures, raw simulation data including the HCACF and thermal conductivity are processed into graph representations and input into a GCN for latent feature extraction. The resulting latent vectors are then passed into a LSTM network, which performs multi-step recursive prediction of future system states. Finally, the predicted latent vectors are decoded into thermal conductivity via a fully connected layer.

References

[1] Feng S H, Chen H F, Zhang J, An M, and Zhang G 2026 *Chin. Phys. Lett.* **43** 020801

*Corresponding authors. Email: anmeng@sust.edu.cn; gangzhang2006@gmail.com

© 2026 Chinese Physical Society and IOP Publishing Ltd. All rights, including for text and data mining, AI training, and similar technologies, are reserved.