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GALAMOST: GPU-accelerated large-scale molecular simulation toolkit

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Software

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Summary

GPU-Accelerated LArge-scale MOlecular Simulation Toolkit (GALAMOST) is a versatile molecular dynamics simulation package which is designed to utilize the computational power of graphics processing units (GPUs) at the state-of-the-art level(Y.-L. Zhu and H. Liu and Z.-W. Li and H.-J. Qian and G. Milano and Z.-Y. Lu, 2013)(Y.-L. Zhu and D. Pan and Z.-W. Li and H. Liu and H.-J. Qian and Y. Zhao and Z.-Y. Lu and Z.-Y. Sun, 2018).

This package is developed specially for large-scale simulations by combining high-performance computation techniques and innovative coarse-graining models and methods(H. Liu and Y.-L. Zhu and Z.-Y. Lu and F. Müller-Plathe, 2016)(W. D. Chen and Y. L. Zhu and F. C. Cui and L. Y. Liu and Z. Y. Sun and J. Z. Chen and Y. Q. Li, 2016)(Z.-W. Li and Y.-L. Zhu and Z.-Y. Lu and Z.-Y. Sun, 2018). Moreover, the multi-scale simulations are supported by implementing all-atom and bottom-up coarse-graining simulations, where involved methods including virtual interaction site, LINCS bond constraint, numerical potential, etc. have been included. Notably, all functionalities are based on pure GPU computation. The package could be employed to study the self-assembly of small and giant molecules, the structure and phase behaviors of liquid crystals, the properties related to polymerization, etc. GALAMOST enriches the routes for researchers to investigate soft matter systems via computer simulations for obtaining advanced materials. The package is written with C++ and CUDA C languages. Python scripts provide the user interface with some examples. Website provides stable packages and user's manual. Unique and common features of GALAMOST are listed.

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