Li ion diffusion in solid electrolyte analyzed using deep generative models.

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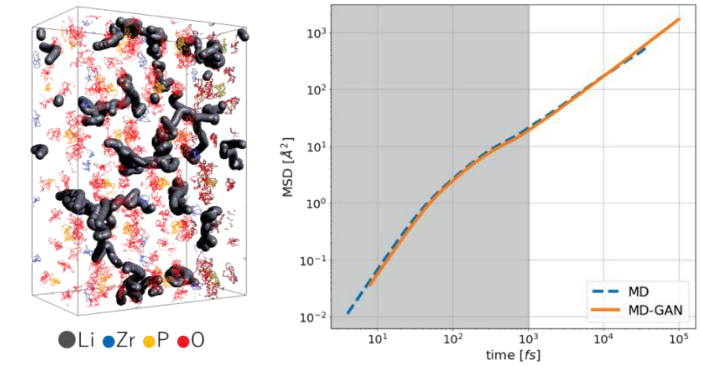
Abstract

Molecular Dynamics (MD) are effective in investigating materials properties at the atomic level, however, the computational costs are notably high, particularly when using ab-initio MD (AIMD). Even as parallelization techniques have expanded the spatial scale of MD, the extension of the temporal scale remains a persisting challenge.

New computational approaches, particularly those incorporating machine learning are gaining traction for accelerating computation. Machine learning potential is one of the technologies for efficient computation with ab-initio levels accuracy. MD-GAN [1,2,3] is another option to utilize machine learning technique in molecular simulation. MD-GAN, based on Generative Adversarial Networks (GAN), has the potential to generate long-term data from short-term data. To minimize computational costs, it is essential to keep the duration of MD calculations, utilized as training data, as short as possible. We have investigated the accuracy and optimal conditions of MD-GAN when applied to prediction of Li ion diffusion in a solid electrolyte system (LZP) [4] obtained using AIMD with SIESTA code [5]. We have confirmed the mean square displacement predicted by MD-GAN agreed well with results of AIMD as shown in the below figure. Furthermore, we have examined the effects on accuracy as the length of input data is shortened with increasing number of trajectories, aiming to reduce the number of MD calculation steps for MD-GAN training. This leads to faster computation through temporal parallelization.



References

[1] Endo, K., Tomobe. K. and Yasuoka, K., Proceedings of the AAAI Conference on Artificial Intelligence, 32, 2192 (2018).

[2] Kawada, R., Endo, K., Yasuoka, K., Kojima, H. and Matubayasi, N., Journal of Chemical Information and Modeling, 63, 76-86 (2022).

[3] Kawada, R., Endo, K., Yuhara, D. and Yasuoka, K, Soft Matter, 18, 8446-8455 (2022).

[4] Fukuya, T., Nitta, H., Ozawa, T., and Yasuoka, K., AIChE 2023 Annual Meeting