SORTING CATEGORY: 16 General Theory, Computational Physics (DCOMP)

SUB CATEGORY TYPE: 16.01.04 Machine Learning for Electronic Structure, Properties and Dynamics of Molecules and Materials

TITLE: First-principles study of THz dielectric properties of molecular liquids with a machine learning model for dipole moments

NAME: Tomohito Amano, Tamio Yamazaki, Shinji Tsuneyuki

ABSTRACT:

The dielectric response of materials in the THz region has been studied extensively in recent years due to improvements in experimental techniques and increased industrial interest. Dipole moments are collected along a molecular dynamics trajectory to calculate the dielectric response from linear response theory. Therefore, it is necessary not only to get accurate trajectories but also to calculate dipole moments precisely [1]. Recently, machine learning for dipole moment has been studied using the centroid of Wannier functions for molecules [2,3] with Wannier functions obtained from first-principles calculations as training data. We have constructed a versatile machine-learning model of dipole moments applicable to molecular liquids. We assigned Wannier functions to chemical bonds between atoms and used deep neural networks to predict the position of the Wannier function for each bond, which is applicable to complex materials. We applied our method to calculate the dielectric function of liquid methanol, and the results were in good agreement with experiments.

[1] C. C. Wang, J. Y. Tan, and L. H. Liu, AIP Advances 7, 035115 (2017).

[2] A. Krishnamoorthy, K. Nomura, N. Baradwaj et al., Phys. Rev. Lett. 126, 216403 (2021).

[3] L. Zhang, M. Chen, X. Wu et al., Phys. Rev. B 102, 041121 (2020).