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

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

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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. Theoretically, the dielectric response is calculated from dipole moments collected along a molecular dynamics trajectory. Therefore, it is necessary not only to get accurate trajectories but also to calculate dipole moments precisely [1]. Recently, machine learning of molecular dipole moments has been studied using the centroid of Wannier functions calculated from first principles[2,3]. 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 the calculation of the dielectric function of liquid alcohols and obtained the results showing good agreement with the experimental ones.

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[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).