

March 15, 2020

Dear Editor,

Here we are submitting our manuscript entitled “Understanding plasmon dispersion in nearly-free-electron metals: the relevance of exact constraints for novel exchange-correlation kernels within time-dependent density functional theory”, by N.K. Nepal, S. Adhikari, B. Neupane, S. Ruan, S. Neupane, and A. Ruzsinszky.

Plasmon dispersion is an interesting physical problem that challenges theory. Before moving toward applications, we aim to understand the basis physics of plasmon dispersion. In order to do this, we use time-dependent density functional theory (TDDFT). Exchange-correlation effects on the linear response function in TDDFT are incorporated by the exchange-correlation kernels. These static exchange-correlation kernels usually have a large impact on the ground state correlation energy. Within this work, we want to investigate what impact these kernels have on plasmon dispersion of nearly-free electron metals such as Cs. The negative dispersion of real Cs can be obtained by calculations that include the effect of the band structure. The impact of the correlation is not obvious, and since the early 2000’s not much improvement has been demonstrated with model kernels that could potentially show the effect of correlation. To decouple band structure and correlation effects, we resort to the simple but predictive jellium model. Our work aims to fill this gap and provides a novel insight: why negative dispersion cannot be obtained without the band structure.

Your consideration of our manuscript as a regular article is highly appreciated.

Sincerely,

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