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Material Specific Exchange-Correlation Kernel Across Jacob's Ladder and Temperature Regimes

We developed a new method [1] that allows one to compute material specific static exchange-correlation (XC) kernel across temperature regimes using standard DFT codes and for any XC functional available in Libxc. We show the results of the static exchange-correlation kernel analysis using various XC functionals for dense electron gas and warm dense hydrogen. By comparing the data to the exact QMC results, we are able to understand the effect of thermal excitations and density inhomogeneity on the exchange-correlation kernel. Moreover, we discuss the results of the analysis of the accuracy of the commonly used XC functionals for warm dense matter simulations [2-6]. The analysis is performed by comparing path-integral quantum Monte-Carlo (QMC) data with KS-DFT results. The application of this methodology for linear response time-dependent DFT calculations is discussed as well [7,8].

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