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Ab Initio Static Exchange–Correlation Kernel From DFT

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The KS-DFT is the standard method to model the electronic structure due to its accuracy and computational efficiency. The reduction in computation cost compared to other ab initio methods is due to a formally exact mapping onto an effective single-electron problem. DFT calculations of a various material properties require as input the so-called exchange—correlation (XC) kernel. Yet, little is known about the actual kernel of real materials, and hitherto no reliable universal way to compute it has been known. In this work, we present a new methodology to compute the static XC-kernel of any material; which needs no external input apart from the usual XC-functional. The application of the method is demostrated for the uniform electron gas and hydrogen. Moreover, we consider both ambient conditions and the warm-dense matter (WDM) parameters. In addition, our analysis of the static XC-kernel gives us valuable new insights into the construction of the XC-functionals for the application at WDM regime.

Primary author: MOLDABEKOV, Zhandos (CASUS, Helmholtz-Zentrum Dresden-Rossendorf, Germany)

Presenter: MOLDABEKOV, Zhandos (CASUS, Helmholtz-Zentrum Dresden-Rossendorf, Germany)

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