Ab Initio Thermodynamic Results for the Degenerate Electron Gas at Finite Temperatures TIM SCHOOF, TOBIAS DORNHEIM, SIMON GROTH, Kiel University, JAN VORBERGER, Helmholtz-Zentrum Dresden-Rossendorf, MICHAEL BONITZ, Kiel University — Recent advances in warm dense matter physics, e.g. laser compressed matter, lead to an increasing interest in the description of correlated, degenerate electrons at finite temperatures. The uniform electron gas (UEG) is of key relevance for the understanding of such systems. Accurate thermodynamic data for the UEG are essential for the development of the finite-temperature density functional theory (FT-DFT).
Based on first principles, the Configuration PIMC approach (CPIMC) allows for the exact computation of thermodynamic properties of strongly degenerate fermionic many-body systems in the highly degenerate regime [1]. We present CPIMC exchange-correlation energies for the UEG [2] and compare our results with previous restricted path integral Monte Carlo (RPIMC) [3] and recently published permutation-blocking PIMC (PB-PIMC) [4] data. We show that the complementary sign problem of the CPIMC and PB-PIMC methods allows for results with an unprecedented accuracy in a wide range of temperatures and densities.
[1] Contrib. Plasma Phys. **51**, 687 (2011).
[2] Phys. Rev. Lett. **115**, 130402 (2015).
[3] Phys. Rev. Lett. **110**, 146405 (2013).
[4] arXiv:1508.03221 (2015).

Tim Schoof
Kiel University