Contribution ID: **8** Type: **not specified**

Conditional probability DFT and warm dense matter

Friday 16 September 2022 09:45 (45 minutes)

Recently, our group suggested an alternative approach to standard DFT calculations. In CP-DFT, we use Kohn-Sham calculations to find conditional probability densities at every point in a system. These are then integrated to yield the exchange-correlation energy, thereby avoiding the need (and many of the failures) to find the energy via an approximate functional. We found that we could reproduce (reasonably accurately) the uniform gas ground-state energy and free energy as a function of temperature, as well as having no self-interaction error for one-electron systems, and being able to correctly dissociate the H2 molecule. I will summarize our progress toward using this to generate the temperature dependence of PBE.

[1] Bypassing the Energy Functional in Density Functional Theory: Direct Calculation of Electronic Energies from Conditional Probability Densities Ryan J. McCarty, Dennis Perchak, Ryan Pederson, Robert Evans, Yiheng Qiu, Steven R. White, and Kieron Burke, Phys. Rev. Lett. 125, 266401 (2020).
[2] Correlation energy of the uniform gas determined by ground state conditional probability density functional theory Dennis Perchak, Ryan J. McCarty, and Kieron Burke, Phys. Rev. B 105, 165143 (2022).
[3] Conditional probability density functional theory Ryan Pederson, Jielun Chen, Steven R. White, and Kieron Burke, to appear in Phys Rev B (2022).

Primary author: BURKE, Kieron (University of California, Irvine, United States)

Co-author: KOZLOWSKI, John

Presenter: BURKE, Kieron (University of California, Irvine, United States)

Session Classification: Morning Session (Friday)