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Basics of electron structure DFT in chemistry, condensed-matter, and materials science: From the very fundamental to the very latest (machine-learning)

Tuesday, 20 June 2017 09:30 (1h 15m)

In the first half of my talk, I will explain how DFT has become the standard method for performing electronic structure calculations in many fields, with over 30,000 papers applying DFT each year[1,2]. In the second half, I will discuss some very recent results from very different approaches: The semiclassical origins of DFT[3], and functionals found by machines[4,5].

[1] DFT in a nutshell Kieron Burke, Lucas O. Wagner, Int. J. Quant. Chem. 113, 96-101 (2013).
[2] DFT: A Theory Full of Holes? Aurora Pribram-Jones, David A. Gross, Kieron Burke, Annual Review of Physical Chemistry 66, 283-304 (2015).
[3] Corrections to Thomas-Fermi Densities at Turning Points and Beyond Raphael F. Ribeiro, Donghyung Lee, Attila Cangi, Peter Elliott, Kieron Burke, Phys. Rev. Lett. 114, 050401 (2015).
[4] By-passing the Kohn-Sham equations with machine learning Felix Brockherde, Leslie Vogt, Li Li, Mark E Tuckerman, Kieron Burke, Klaus-Robert M uller, (submitted) (2016).
[5] Pure density functional for strong correlation and the thermodynamic limit from machine learning Li Li, Thomas E. Baker, Steven R. White, Kieron Burke, Phys. Rev. B 94, 245129 (2016).

Presenter: Prof. BURKE, Kieron (UC Irvine)