

The exact functional of density functional theory

Aron J. Cohen^a and Paula Mori-Sánchez^b

^a *Department of Chemistry, University of Cambridge, Cambridge, CB2 1EW, UK*

^b *Departamento de Química, Universidad Autónoma de Madrid, 28049 Madrid, Spain*

The proof of the existence of the exact functional, $F[\rho]$ by Hohenberg and Kohn¹ created the entire field of density functional theory (DFT). However, recent development of improved approximations to this functional has not been able to provide chemical accuracy in all cases especially in strongly correlated systems². It is now time to explore all aspects of the exact functional.

By explicitly carrying out the Constrained Search³ in simple model systems such as the Hubbard model and electrons in one-dimension, we will illustrate many features of the exact functional. $F[\rho]$ not only exists, it is something that can be calculated, visualized and in some cases even 3d-printed⁴. We will also show a view of strongly correlated wavefunctions and approaching the strictly correlated limit. We hope to highlight new avenues to the development of novel and improved functionals in DFT.

- [1] P. Hohenberg and W. Kohn, *Phys. Rev.* **136**, B864 (1964).
- [2] A. J. Cohen, P. Mori-Sánchez and W. Yang, *Chem. Rev.* **112** 289 (2012).
- [3] M. Levy, *Proc. Natl. Acad. Sci.* **76** 6062 (1979).
- [4] A. J. Cohen and P. Mori-Sánchez, *Phys. Rev. A* **93** 042511 (2016).