Abstract Submitted
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Density functionals from deep learning JEFFREY MCMAHON, Department of Physics and Astronomy, Washington State University — Density-functional theory is a formally exact description of a many-body quantum system in terms of its density; in practice, however, approximations to the universal density functional (DF) are necessary. Machine learning has recently been proposed as a novel approach to discover such a DF (or components of it)[1]. Conventional machine learning algorithms, however, are limited in their ability to process data in their raw form, leading to invariance and/or sensitivity issues. In this presentation, an alternative approach based on deep learning will be demonstrated[2]. Deep learning allows computational models that are capable of discovering intricate structure in large and/or high-dimensional data sets with multiple levels of abstraction, and do not suffer from the aforementioned issues. Results from the application of this approach to the prediction of the kinetic-energy DF of noninteracting electrons will be presented. Using theoretical results from computer science, a connection between the underlying model and the theorems of Hohenberg and Kohn will also be suggested.

[1]J. C. Snyder, M. Rupp, K. Hansen, K.-R. Müller, and K. Burke, *Phys. Rev. Lett.* **108**, 253002 (2012).
[2]J. M. McMahon, *Submitted* (2015).

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