Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Finding density functionals with machine learning[1] JOHN SNYDER, University of California, Irvine, MATTHIAS RUPP, Eidgenossische Technische Hochschule, Zurich, KATJA HANSEN, KLAUS MUELLER, Technische Universitat, Berlin, KIERON BURKE, University of California, Irvine — Using standard methods from machine learning, we introduce a novel technique for density functional approximation. We use kernel ridge regression with a Gaussian kernel to approximate the non-interacting kinetic energy of 1-dimensional multi-electron systems. With fewer than 100 training densities, we can achieve mean absolute errors of less than 1 kcal/mol on new densities. We determine densities for which our new functional will fail or perform well. Finally, we use principle component analysis to extract accurate functional derivatives from our functional, enabling an orbital-free minimization of the total energy to find a self-consistent density. This empirical method has two parameters, set via cross-validation, and requires no human intuition. In principle, this general technique can be extended to multi-dimensional systems, and can be used to approximate exchange-correlation density functionals.

[1]We thank NSF (CHE-0809859), DFG (MU 987/4-2) and EU (PASCAL2) for support.

John Snyder
University of California, Irvine

Date submitted: 11 Nov 2011 Electronic form version 1.4