Can machines beat humans at electronic structure?

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In this talk, I will discuss a variety of work I'm been involved in, with a focus on using machine learning to find density functionals. The Hohenberg-Kohn theorem guarantees the existence of a universal ground-state density functional, and the Kohn-Sham scheme, with present-day approximations, combines useful accuracy with computational efficiency. Most approximations begin with the local density approximation and DFT has enjoyed tremendous success as well as notorious failures.

I will explain how we have used machine learning to generate more accurate functionals than any constructed by humans, and how this method can overcome problems inherent with our present generation of functionals.

Relevant references may be found at http://dft.uci.edu/publications.php.