I13

Density functional design based on survival of the most transferable

Martin Head-Gordon
University of California Berkeley

I shall discuss progress in the design of a next generation of density functional theories, including methods at rungs 3, 4, and 5 of Perdew's Jacob's Ladder. In contrast to most approaches to functional design, we have adopted a combinatorial approach, in which we have trained a huge number of functionals (over 10 billion in the case of meta GGA functionals). The functional from each class that performs best on independent test data (survival of the most transferable) is self-consistently trained to yield new generation functionals that seems very promising for application purposes. A key component of these functionals is the non-local VV10 density-density correlation functional that enables highly accurate treatment of non-bonded interactions, if the entire functional is self-consistently trained. The resulting optimal functionals involve far fewer parameters than the maximum permitted in the combinatorial searches. I shall discuss the results of large-scale benchmarking exercises that assess the new functionals against other existing functionals.