Title: **Advances in semi-empirical density functionals for molecules and materials**

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Abstract:

I shall discuss progress in the design of a next generation of density functional theories. 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 100,000 in the case of the generalized gradient approximation models, and over 10^{10} 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 functionals involve significantly fewer parameters than many of the best functionals of recent years. I shall discuss the results of large-scale benchmarking exercises that assess the new functionals against other existing functionals.