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Retrofit of the HSE density functional[1] JONATHAN MOUSSA, PETER SCHULTZ, Sandia National Labs, JAMES CHELIKOWSKY, UT Austin — The original parameterization of the Heyd-Scuseria-Ernzerhof (HSE) density functional was dependent on the choice of a hybrid fraction and a range-separation length for separating out a portion of the exchange energy to compute exactly. For backward compatibility with the PBE0 functional, the hybrid fraction was fixed to 0.25. Here, we examine the full hybrid fraction / separation length phase space. With respect to multiple error metrics, the phase space does not have a well-developed point of minimum error. Instead, there is a "valley" of functionals with increasing hybrid fraction and decreasing separation length of similarly good quality. This enables a reduction of the separation length without degrading the accuracy of the HSE06 parameterization, which in turn reduces the computational cost of evaluating the exchange energy.

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