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Semi-Local DFT Functionals with Exact-Exchange-Like Features: Beyond the AK13[1] RICKARD ARMIENTO, Linkoping Univ - Linkoping — The Armiento-Kümmel functional from 2013 (AK13) [1] is a non-empirical semi-local exchange functional on generalized gradient approximation form (GGA) in Kohn-Sham (KS) density functional theory (DFT). Recent works have established that AK13 gives improved electronic-structure exchange features over other semi-local methods, with a qualitatively improved orbital description and band structure. For example, the Kohn-Sham band gap is greatly extended, as it is for exact exchange. This talk outlines recent efforts towards new exchange-correlation functionals based on, and extending, the AK13 design ideas. The aim is to improve the quantitative accuracy, the description of energetics, and to address other issues found with the original formulation. [1] R. Armiento and S. Kümmel, Phys. Rev. Lett. 111, 036402 (2013).

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