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Exchange-Correlation Potentials from Electronic Wave Functions

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We have developed a method for constructing exchange-correlation potentials, $v_{\rm XC}(\mathbf{r})$, of the Kohn–Sham density-functional theory from *ab initio* many-electron wave functions. In this method, a system-specific Kohn–Sham potential is obtained not by fitting to a given electron density but by using a certain exact expression for $v_{\rm XC}(\mathbf{r})$ in terms of wave-function and Kohn–Sham quantities. The key advantages of this approach are that (i) it is very robust numerically and (ii) when implemented using a finite basis set, it produces accurate approximations to the exact (basis-set-limit) $v_{\rm XC}(\mathbf{r})$ without any basis-set artifacts of Kohn–Sham inversion and optimized-effective-potential techniques. I will explain our approach and illustrate it with numerical examples.

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