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The derivative discontinuity of the exchange-correlation functional

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The derivative discontinuity is a fundamental feature of the exchange-correlation energy. It is the change in the derivative of the energy as the number of electrons goes through an integer, and it is often expressed as a potential that jumps by a constant on going from $N-\delta$ to $N+\delta$. In this talk we will show manifestations in the total energy of integer systems at fixed N. One manifestation is the complete failure of all functionals in the literature to give the energy of **both** infinitely stretched H_2^+ and infinitely stretched H_2. Another very clear example is the failure to correctly reproduce the density in a two electron H_2 like system when changing the charge of one of the protons to be non-integer. More examples in chemistry and physics will be shown, ranging from the behaviour of electrons in the simplest chemical reactions to the gap of the 1D-Hubbard model and electron transport in the Anderson model. To understand the derivative discontinuity in these systems it is important to consider three perspectives, (1) the true behaviour of electrons which can be found by an exact FCI calculation (2) the failures of most currently used approximate functionals, which are all missing the derivative discontinuity (3) investigating new functionals that may have some aspects of the derivative discontinuity. Overall this is a great challenge for $E_{xc}[\rho]$ that must be considered in the development of new functionals.