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Prediction of the derivative discontinuity in density functional theory from an electrostatic description of the exchange and correlation potential

Xavier Andrade, Alán Aspuru-Guzik

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We propose a new approach to approximate the exchange and correlation (XC) functional in density functional theory. The XC potential is considered as an electrostatic potential, generated by a fictitious XC density, which is in turn a functional of the electronic density. We apply the approach to develop a correction scheme that fixes the asymptotic behavior of any approximated XC potential for finite systems. Additionally, the correction procedure gives the value of the derivative discontinuity; therefore it can directly predict the fundamental gap as a ground-state property.

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