

Abstract Submitted
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Partition Theory for Periodic and Semi-Infinite Systems KELSIE NIFFENEGGER, ADAM WASSERMAN, Purdue University — Standard approximations to the exchange-correlation (XC) functional of Kohn-Sham Density-Functional Theory are insufficiently accurate to describe charge transfer at metal-atom interfaces and other systems requiring proper treatment of fractional electron charges. The root of the problem is connected to the lack of derivative discontinuities in the approximate XC functionals at integer numbers of electrons. Partition Theory (PT) is a promising, formally exact method to correct this issue. We study the simplest model for an atom adsorbed at a metal surface: A one-dimensional step potential separated a fixed distance from an attractive well that admits only one bound state when isolated. The semi-infinite metal is populated with non-interacting electrons up to the Fermi energy. We derive the PT-equations for this problem and indicate how the associated partition potential can be calculated. PT is also a promising method for improving the computational scaling of other large and/or periodic systems. We study the partition potential for periodic 1-D chains of identical attractive wells and comment on the uniqueness of the partition potential when going from finite to periodic systems.

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