

Abstract Submitted
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Dimensional crossover of the exchange-correlation energy at the semilocal level¹ LUCIAN CONSTANTIN — Commonly used semilocal density functional approximations for the exchange-correlation energy fail badly when the true two dimensional limit is approached. We show, using a quasi-two-dimensional uniform electron gas in the infinite barrier model, that the semilocal level can correctly recover the exchange-correlation energy of the two-dimensional uniform electron gas. We derive new exact constraints at the semilocal level for the dimensional crossover of the exchange-correlation energy and we propose a method to incorporate them in any exchange-correlation density functional approximation.

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