

Abstract Submitted
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Density Functional Theory for Open Systems¹ ANTONIOS GONIS, Lawrence Livermore National Laboratory, DON NICHOLSON, MALCOLM STOCKS, XIAO GUANG ZHANG, Oak Ridge National Laboratory — We provide a formal proof of the convexity relation, $2E[N] \leq E[N - 1] + E[N + 1]$, characterizing the total energy of interacting N -electron systems under the action of a given external potential, hitherto assumed to be true only on experimental grounds. This is used to prove the inequality, $I(N) - A(N) \geq 0$, where $I(N)$ and $A(N)$ are, respectively, the ionization potential and electron affinity of a N -electron system.

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Xiaoguang Zhang
Oak Ridge National Laboratory

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