

Abstract Submitted
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DC conductance of long molecular chains¹ ROBERTO CAR, EMIL PRODAN, Princeton University — Inspired by the work of Kamenev and Kohn, we obtained a general and formally exact expression for the 2-terminal dc conductance of linear molecular structures, within the framework of Time Dependent Current-Density Functional Theory. In this talk we focus on the adiabatic conductance. For linear molecular chains, both insulating and metallic, we derive exact and asymptotic analytic expressions for the conductance. For insulating chains, for example, not only do we get the exponentially decaying factors, but also the coefficients in front of these factors, which are highly dependent on the contacts. The results are based on the analytic structure of the bands and a compact expression for the Green's functions. Applications will also be presented.

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