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Multi-Step Fisher-Lee: A new tool to predict transport mechanism transition in molecular junctions.

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Abstract:

In the past decade, research groups took advantage of the progress on the growth of molecular junction to explore the electronic transport properties in different regimes (non- resonant tunneling, hopping, resonant-tunneling, etc...) by measuring their electric properties while varying the molecular length[1]. While the existing theories correctly describe the transport in the non-resonant tunneling regime (*i.e.* for short molecules), there is no reliable model to connect the regimes to each other[2]. Here, we present a new methodology based on the Non-Equilibrium Green Function (NEGF) combined to the Fisher-Lee formalism[3] within a semi-classical approach, to predict the transport mechanism transition between the non-resonant tunneling and the following regimes. This new approach labeled Multi-Step Fisher-Lee (MSFL)[4] consists in comparing a direct tunneling mechanism to a multistep tunneling in the Fisher Lee formalism. We have applied it to a wide range of molecular junctions and the obtained results are in a good agreement with experimental measurements. This work opens perspectives for a better understanding of the transport mechanism in molecular junctions.

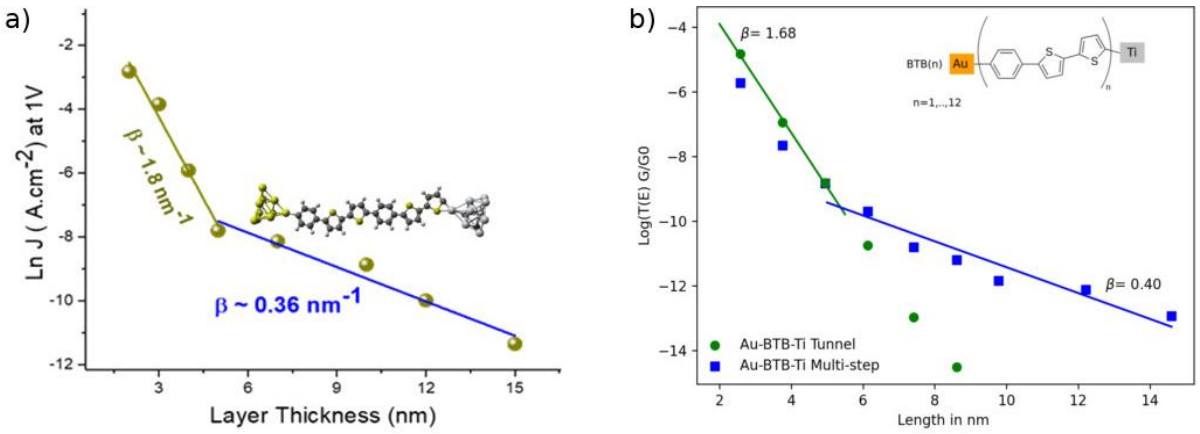

Figure: Comparison of a) experimental[5] results and b) our results using the MSFL method for the molecular junction Au-BTB-Ti.

References:

1. Choi SH *et al*. Transition from Tunneling to Hopping Transport in Long, Conjugated Oligo-imine Wires Connected to Metals. *J Am Chem Soc*. 2010;132(12):4358-4368.
2. Liu H *et al*. Can the transition from tunneling to hopping in molecular junctions be predicted by theoretical calculation? *Journal of computational chemistry*. 2011;32(8):1687-1693.
3. Pitie S *et al*. Fast Fisher-Lee approach for conductance calculations on BTB-based molecular junctions: effects of isomerization and electrode coupling. *Journal of chemical Theory and Computation*. Published online submitted.
4. Pitie S *et al*. A new approach to predic the transport mechanism transition. Published online submitted.
5. Nguyen QV *et al*. Highly Efficient Long-Range Electron Transport in a Viologen-Based Molecular Junction. *Journal of the American Chemical Society*. 2018;140(32):10131-10134.