Elucidating the Shape of the Quantum Tunneling Barrier in Self Assembled Monolayers

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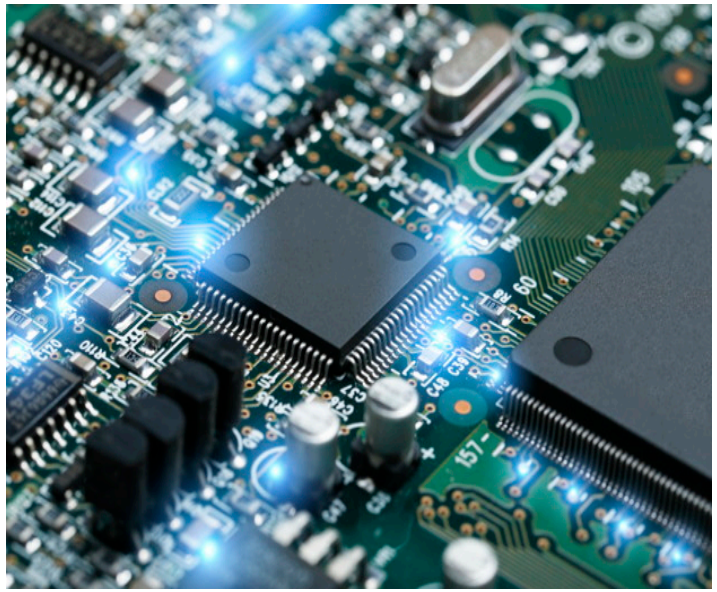
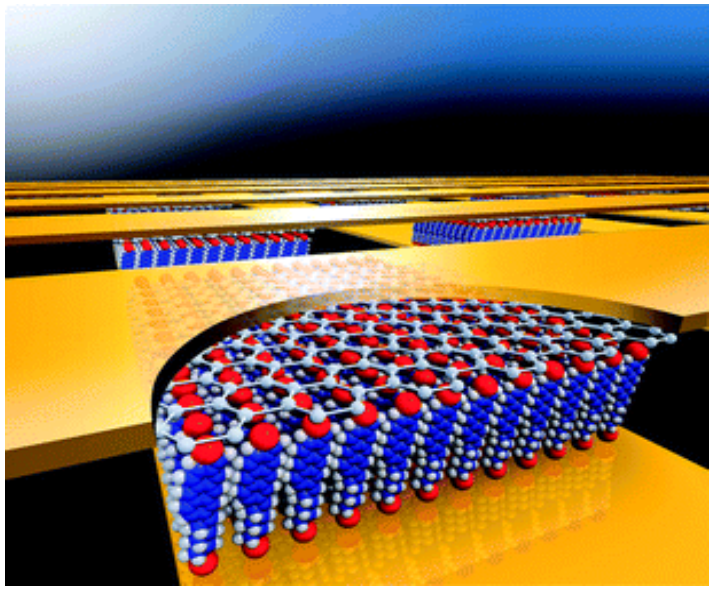
Molecular electronics



http://www.ecmsnews.com/2018/05/24/another-missing-component-revolutionize-electronics/

VS.

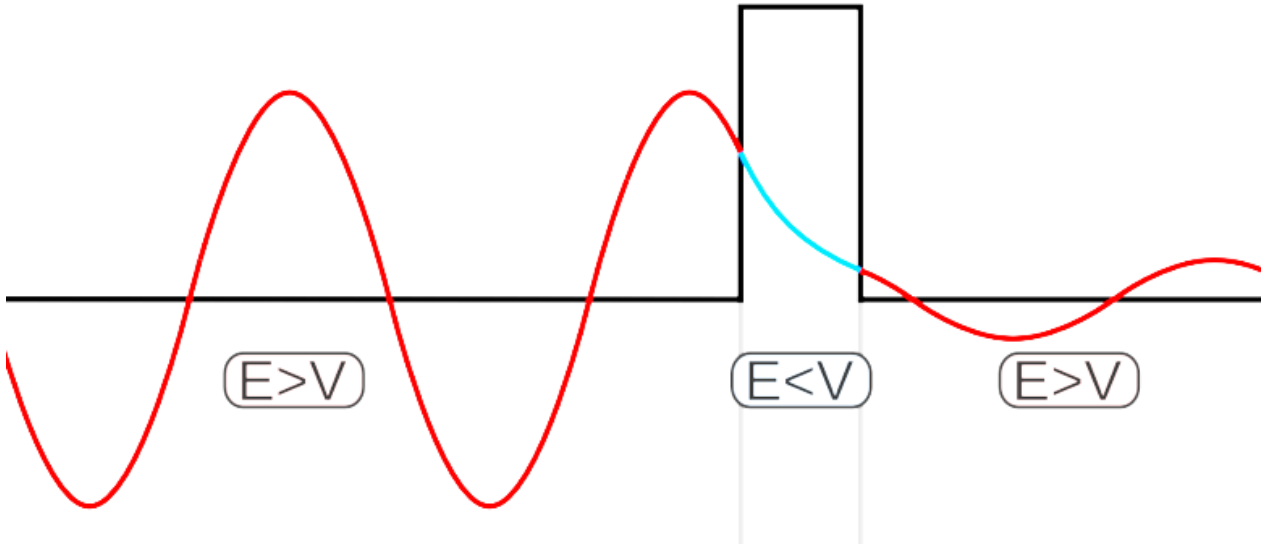


https://www.timetoast.com/timelines/future-of-computers-69ae0e2f-9c3f-4db8-9edf-b32cf4b02068

~ 10 nm

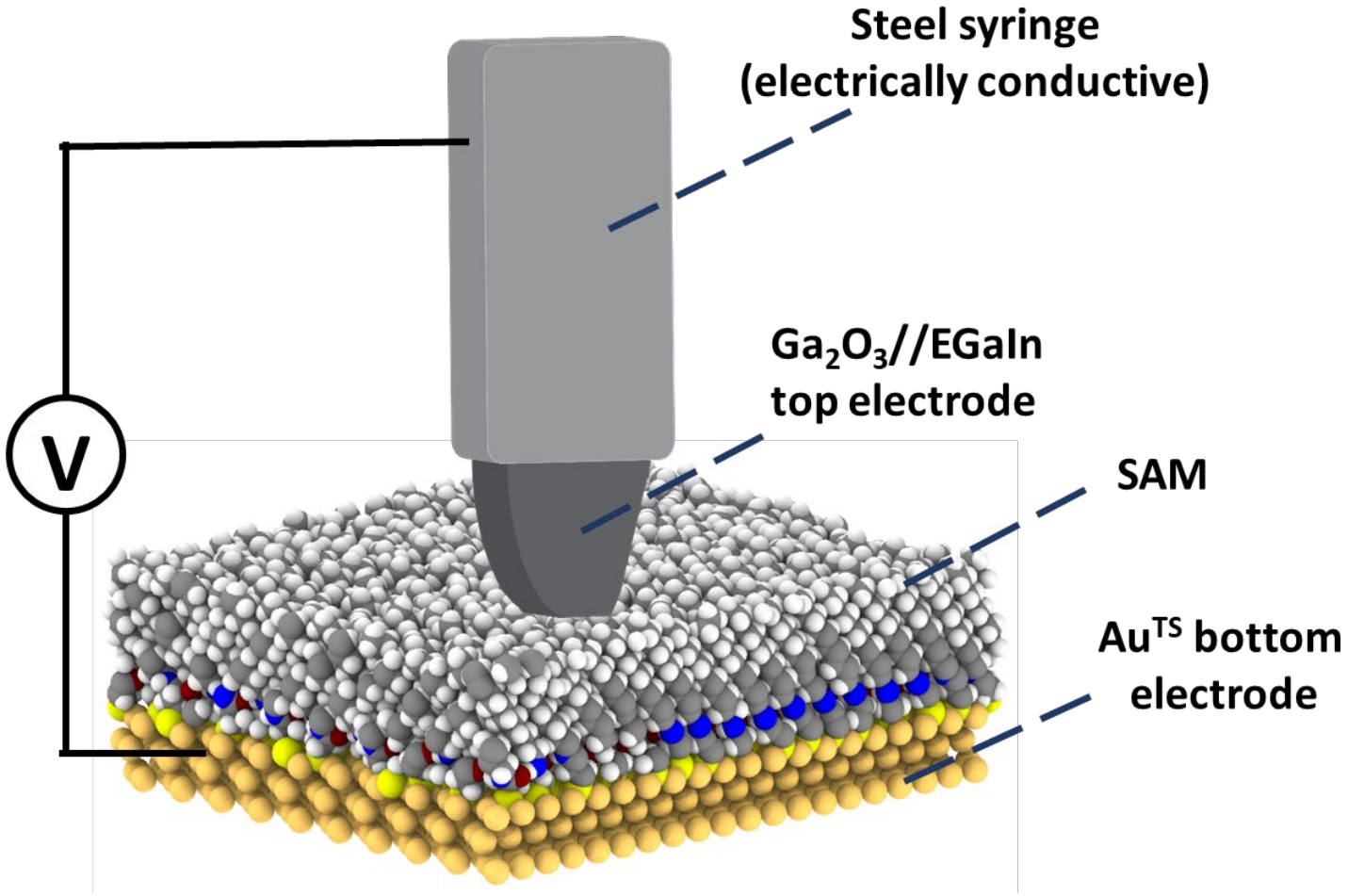
~ 1 nm

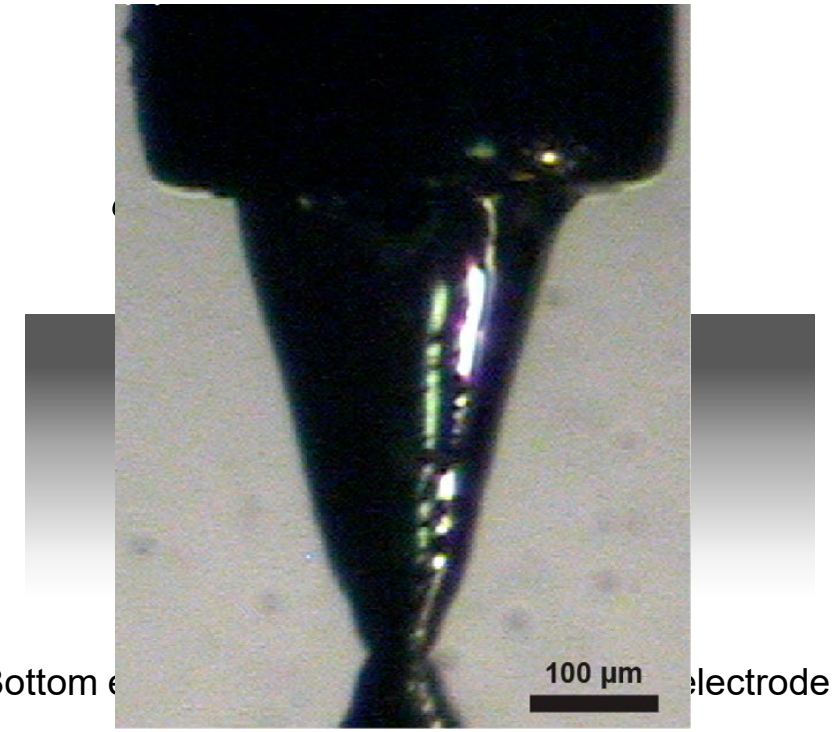
What is quantum tunneling?



Razavy, Mohsen (2003). Quantum Theory of Tunneling. World Scientific

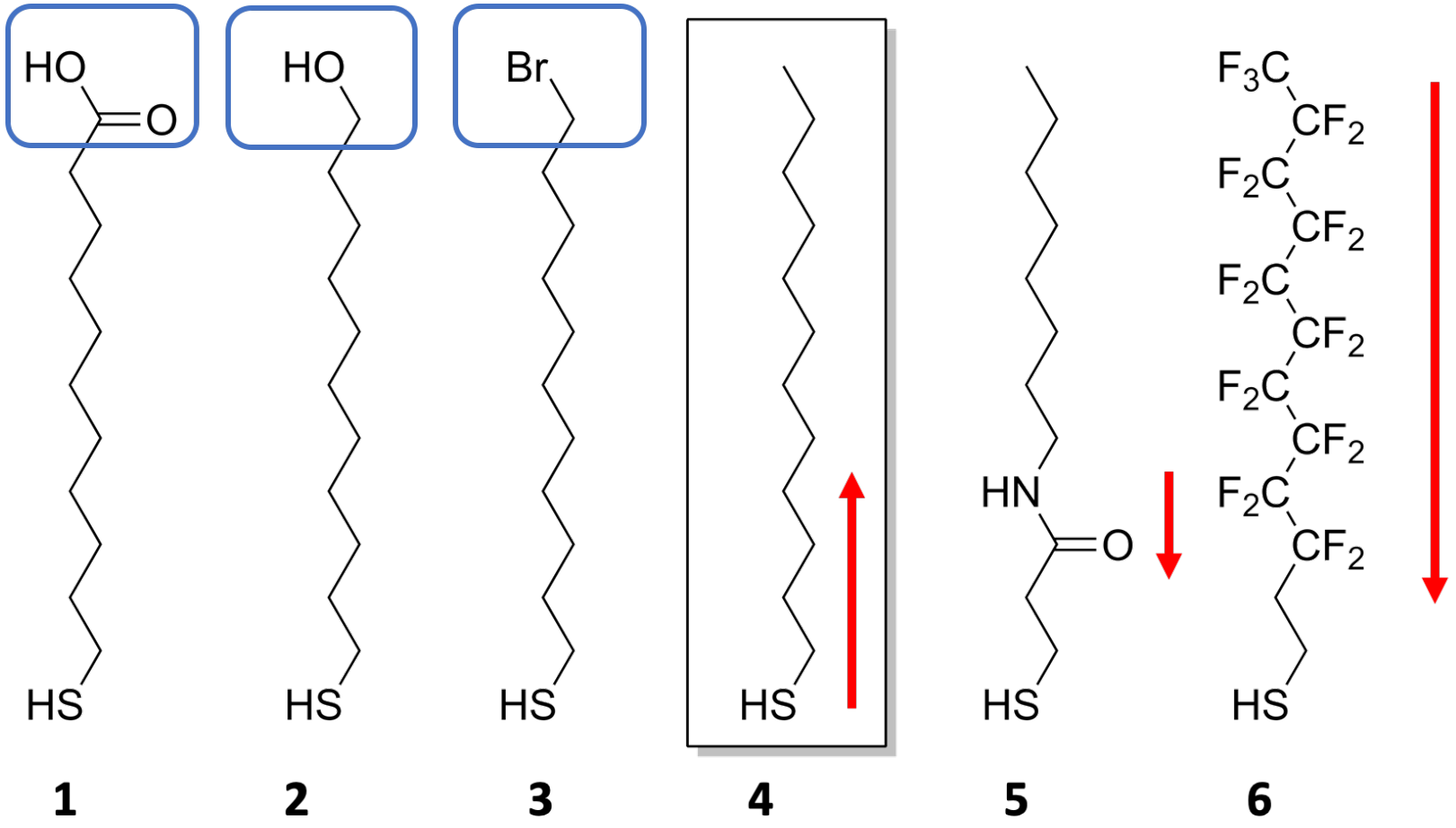
How do we study it?

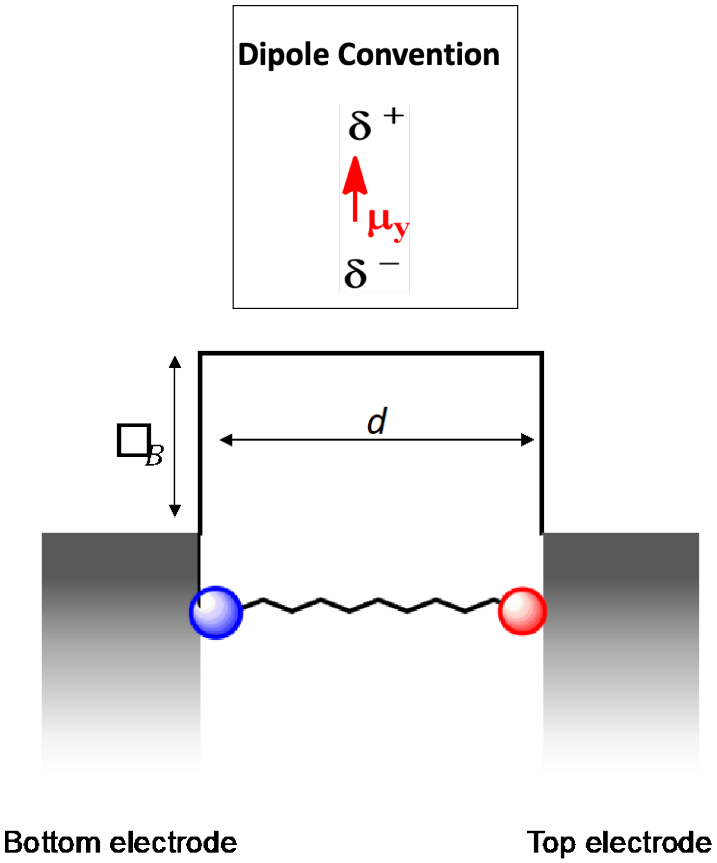




Bottom e lectrode

Molecules we are studying





Effect of terminal groups?

Effect of dipole moment?

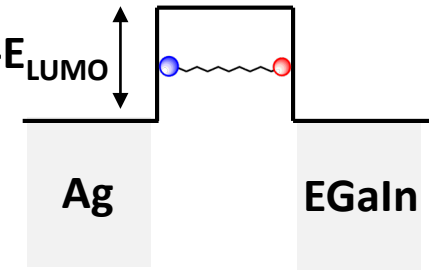
The Tunneling barrier

Direct Tunneling (trapezoidal)

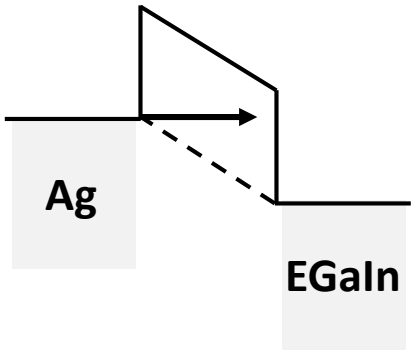
Fowler-Nordheim (F-N) Tunneling (triangular)

$V_{app} = 0$

$\phi = E_{Fermi} - E_{LUMO}$

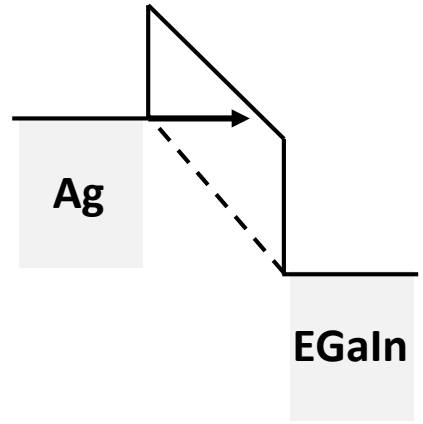


$V_{app} < \phi$



$$J_{DT} \sim V \exp\left(-\frac{2d}{\hbar}\sqrt{2m\Phi_B}\right)$$

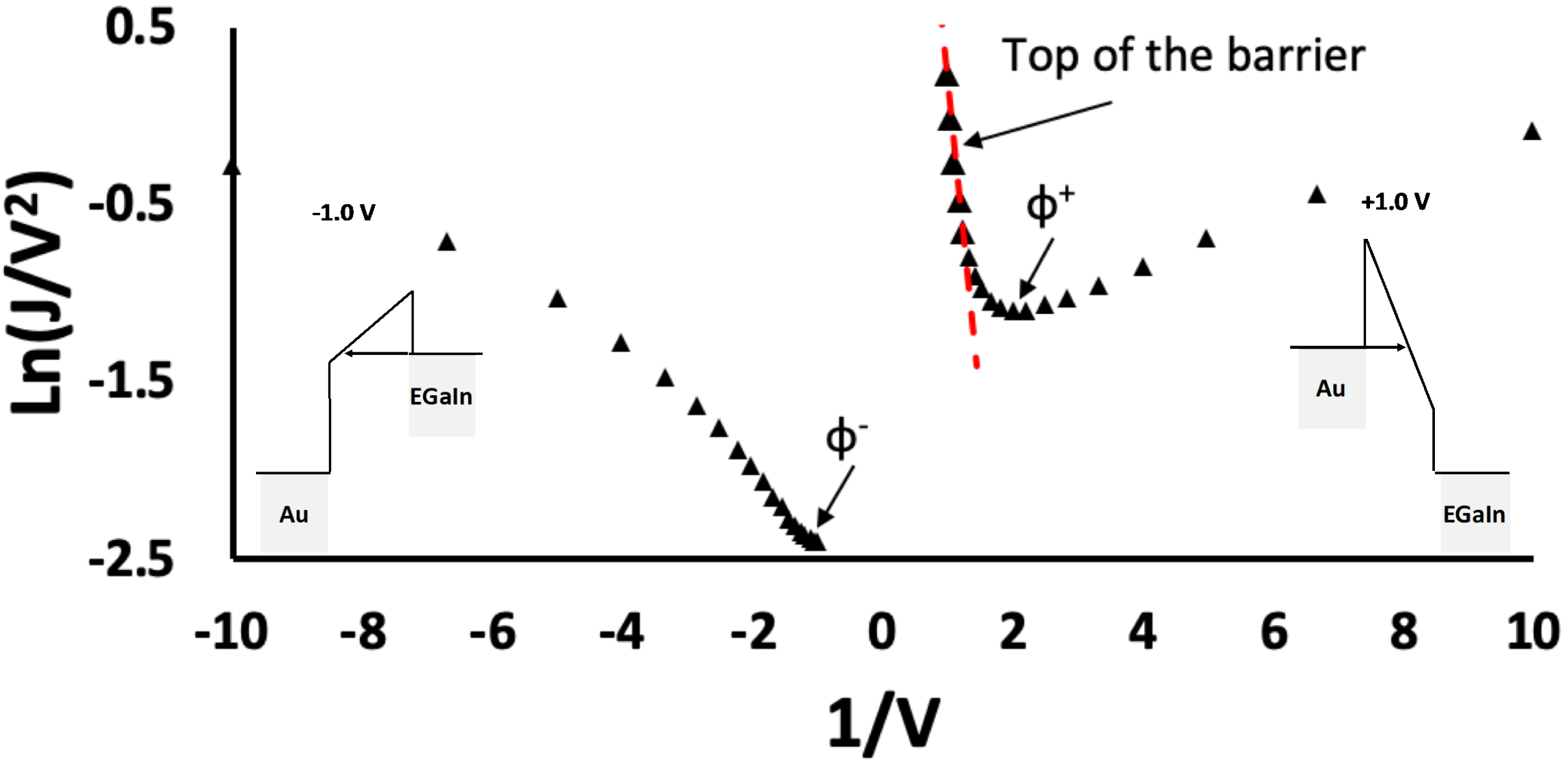
$V_{app} > \phi$

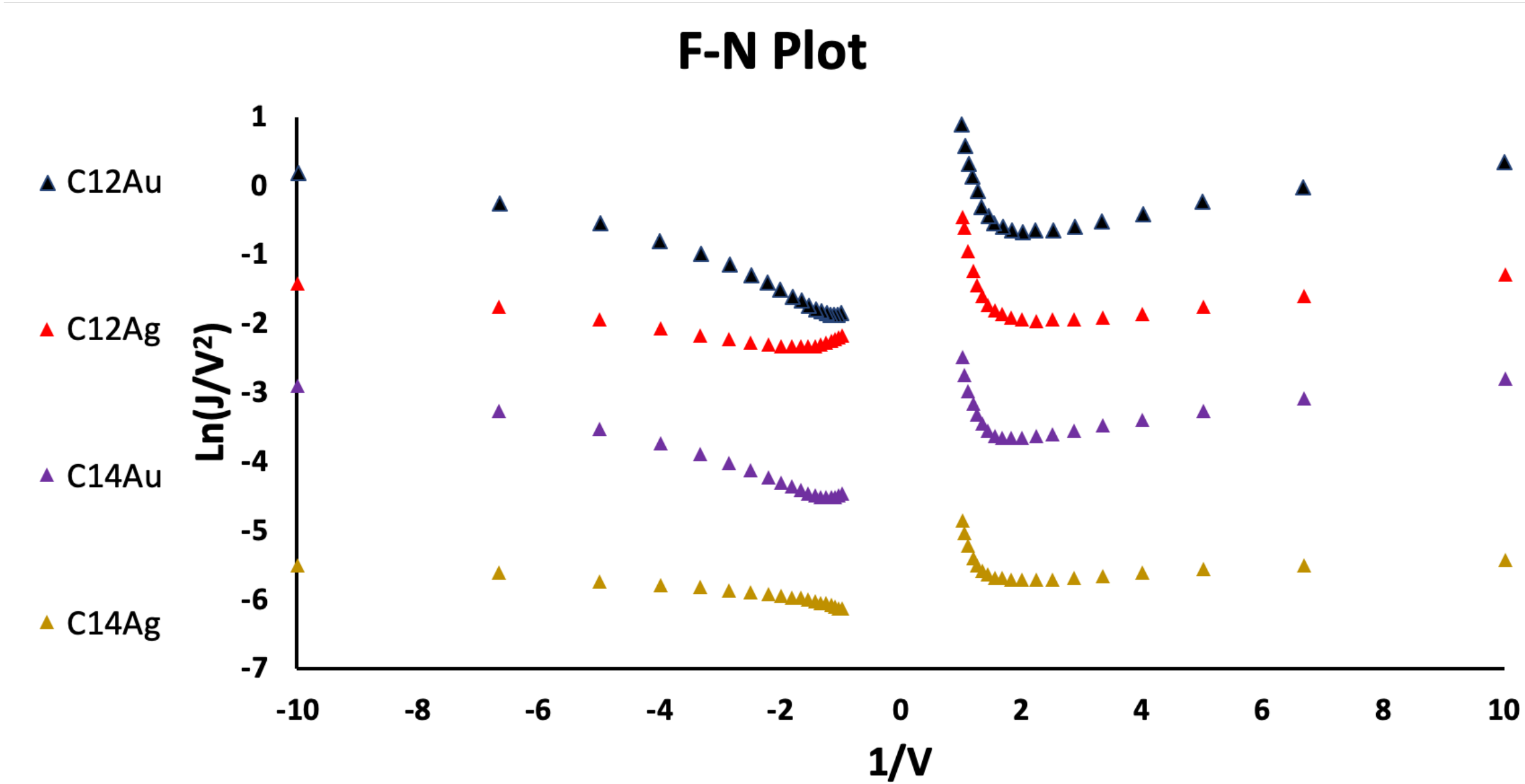


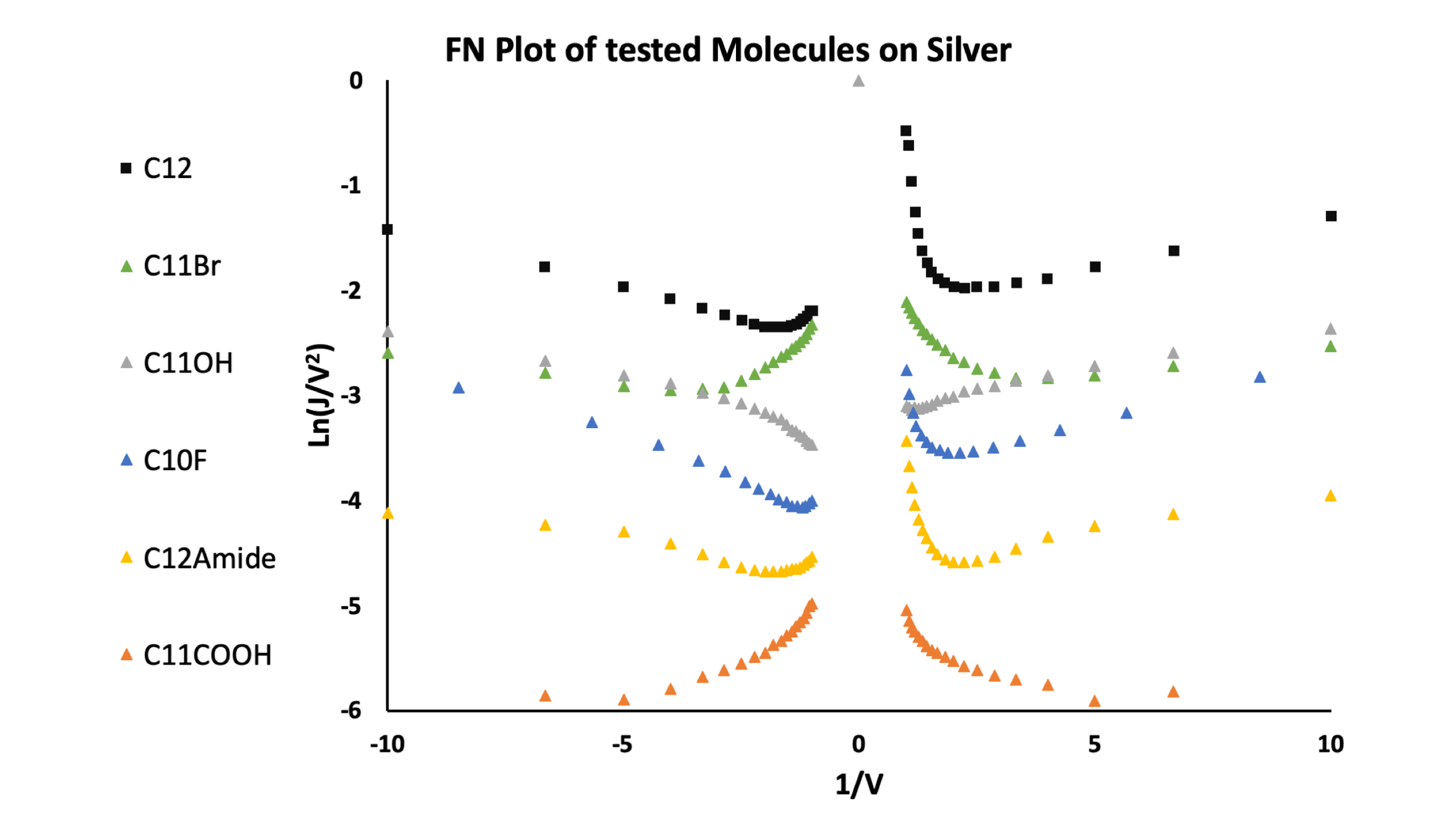
$$J_{FN} \sim V^2 \exp\left(-\frac{4d}{3q\hbar V}\sqrt{2m\Phi_B^3}\right)$$

Phys. Rev. Lett., **97**, 026801 (2006)

F-N Plot of C12 Amide Au

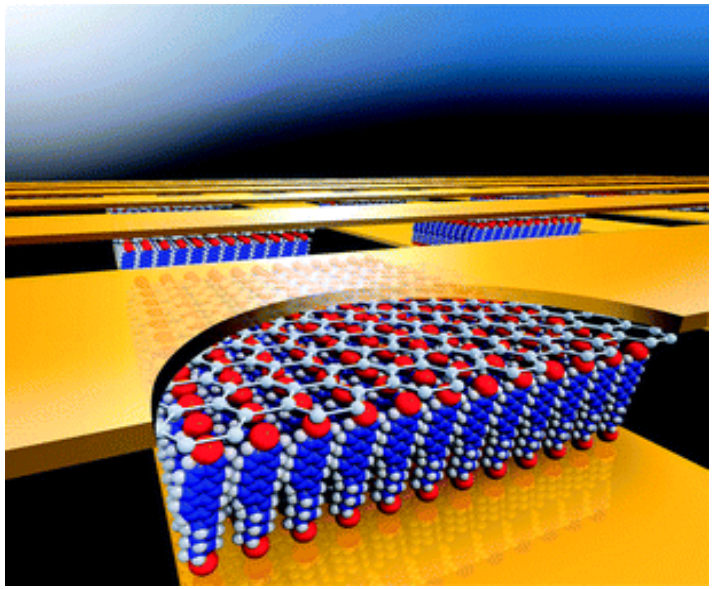



F-N Plot
C12Au
C12Ag
C14Au
C14Ag
Ln(J/V²)
1
0
-1
-2
-3
-4
-5
-6
-7
-10
-8
-6
-4
-2
0
2
4
6
8
10
1/V


FN Plot of tested Molecules on Silver
C12
C11Br
C11OH
C10F
C12Amide
C11COOH
Ln(J/V²)
0
-1
-2
-3
-4
-5
-6
-10
-5
0
5
10
1/V

Conclusion

- Modifications of terminal groups and localized dipoles affect the barrier shape
  - Barrier height
  - Slopes of linear regimes
- The tunneling barrier shape on gold is different than on silver



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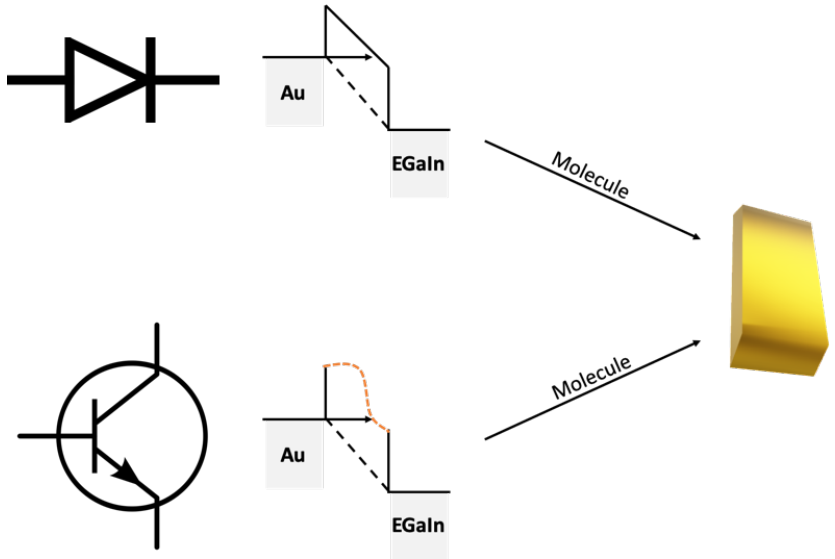
Significance

- Molecular electronics
- Quantum tunneling



Acknowledgments

Dr. Lee Belding

Dr. Junwoo Park

Dr. Sam Root

Dr. Maral Mousavi

Antowan Davtinas

Dr. Alan True

Dr. Kathryn Hollar

Sara Wenzel

Dr. George M. Whitesides

National Nanotechnology Coordinated Infrastructure

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