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Vibrational spectroscopy with functionalized STM tips

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D. Sanchez-Portal, A. Arnau**

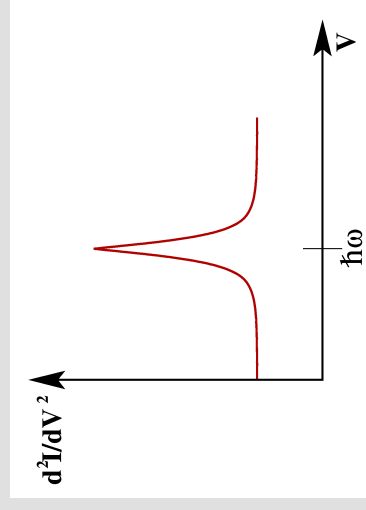
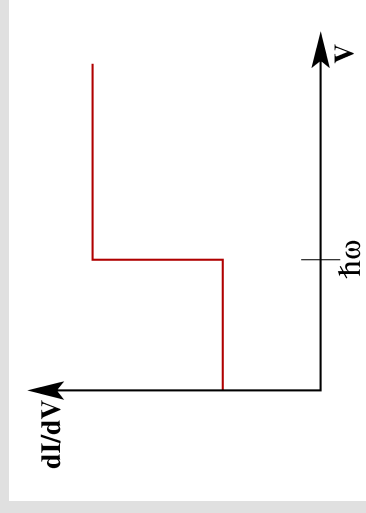
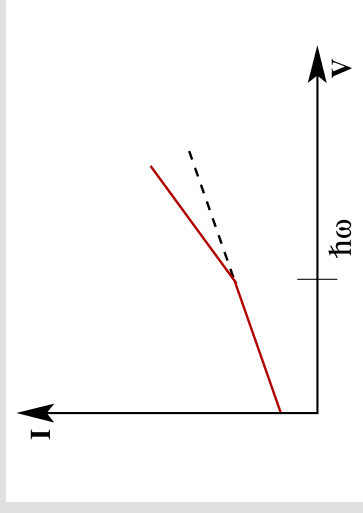
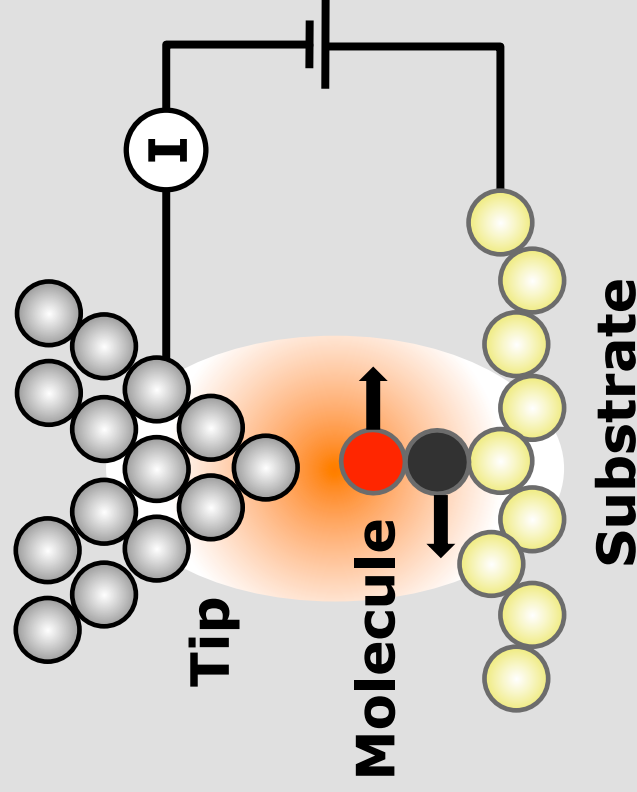


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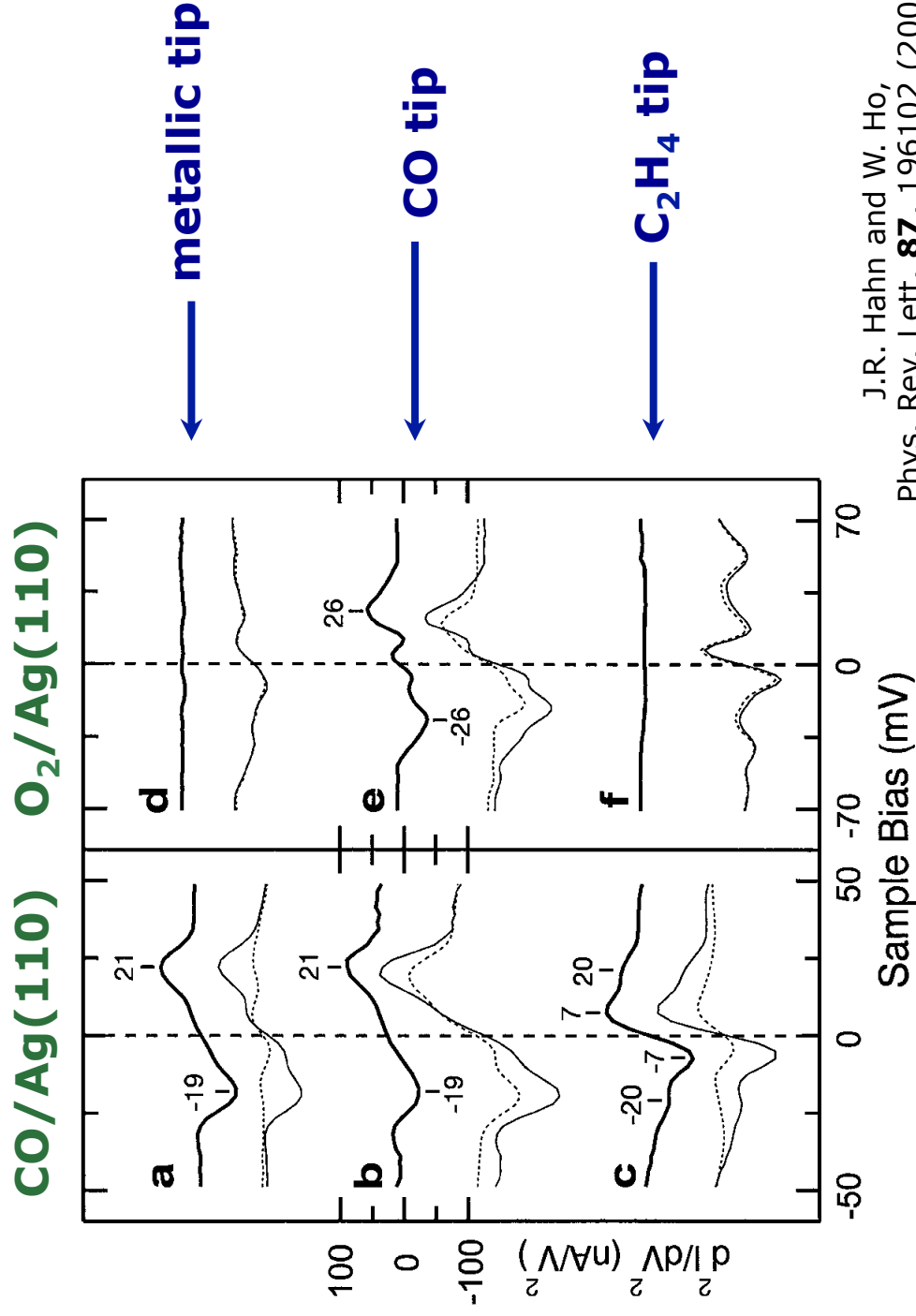


Inelastic Electron Tunneling Spectroscopy (IETS)

Scanning Tunneling Microscope



Limitations of IETS



I

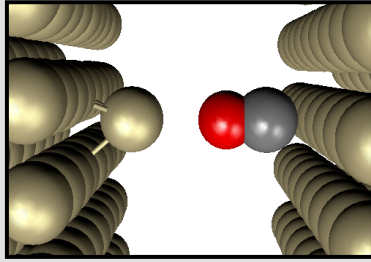
S

J.R. Hahn and W. Ho,
Phys. Rev. Lett. **87**, 196102 (2001)

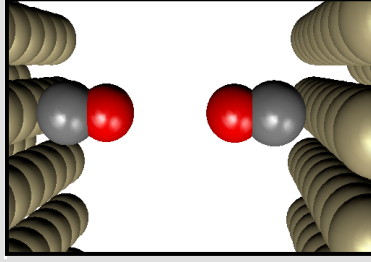
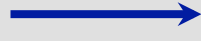
IETS of CO on Cu(111)



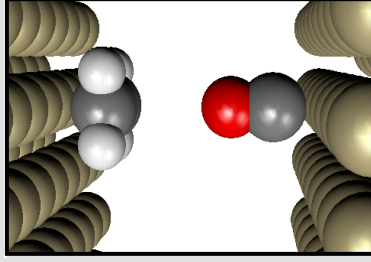
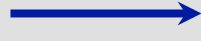
Cu adatom tip



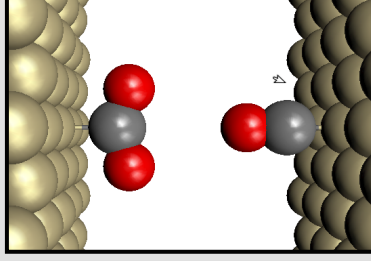
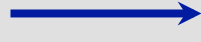
CO tip



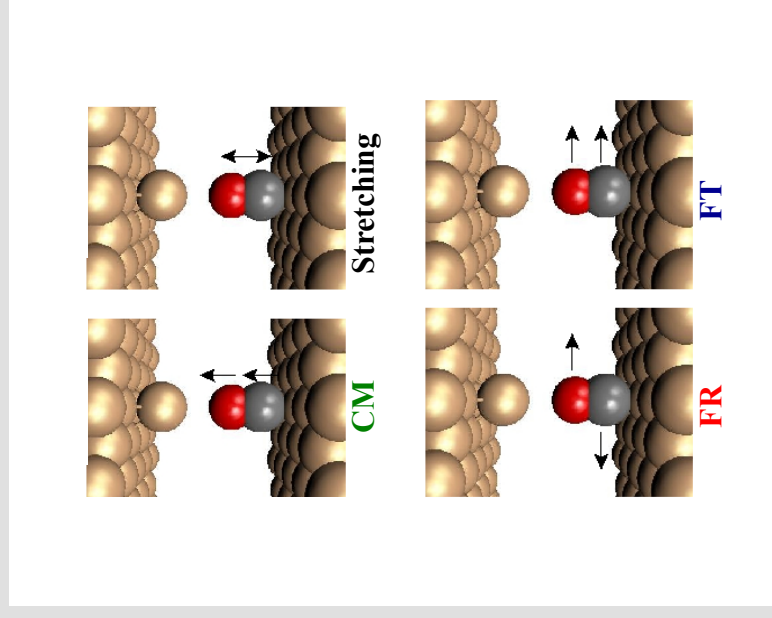
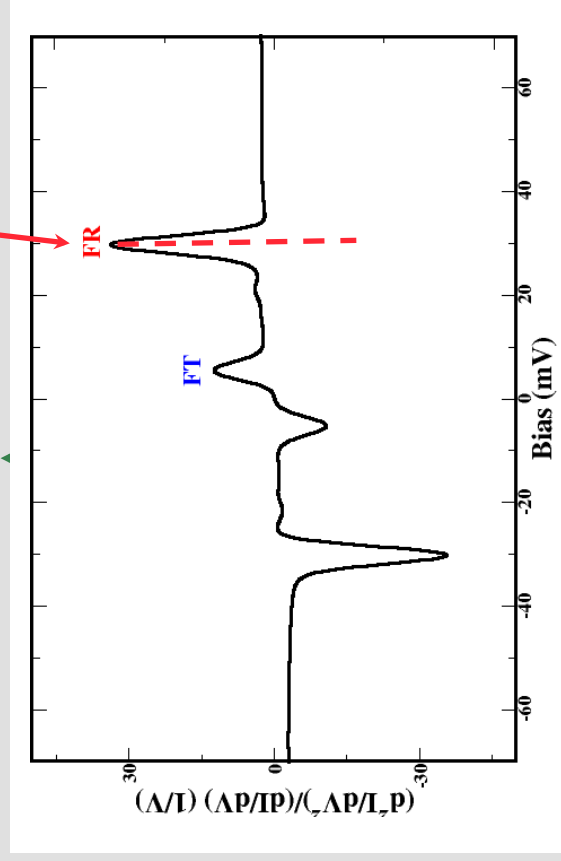
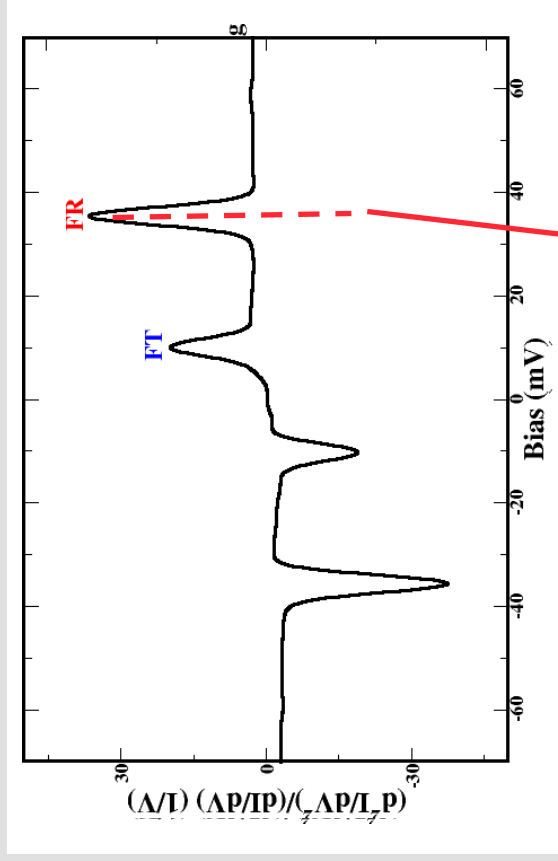
C₂H₄ tip



CO₂ tip



Cu adatom tip

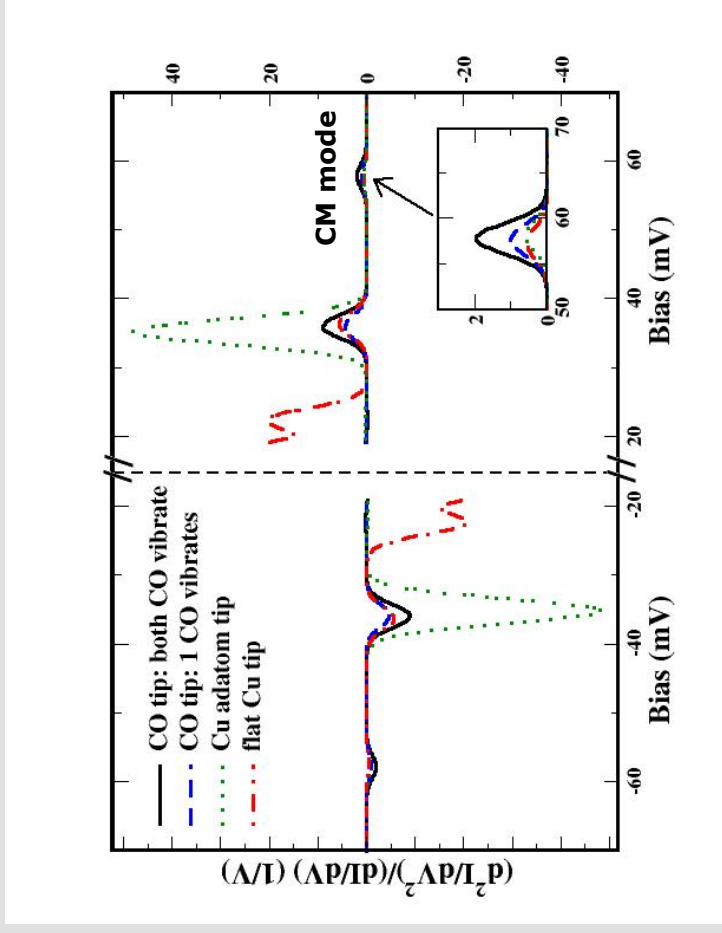
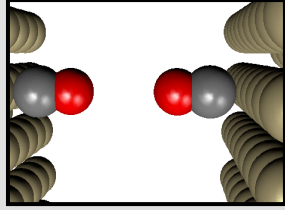


Nanoletters **10**, 657 (2010)

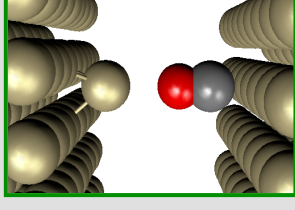
CO tip



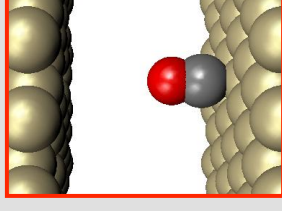
CO tip



Cu adatom tip

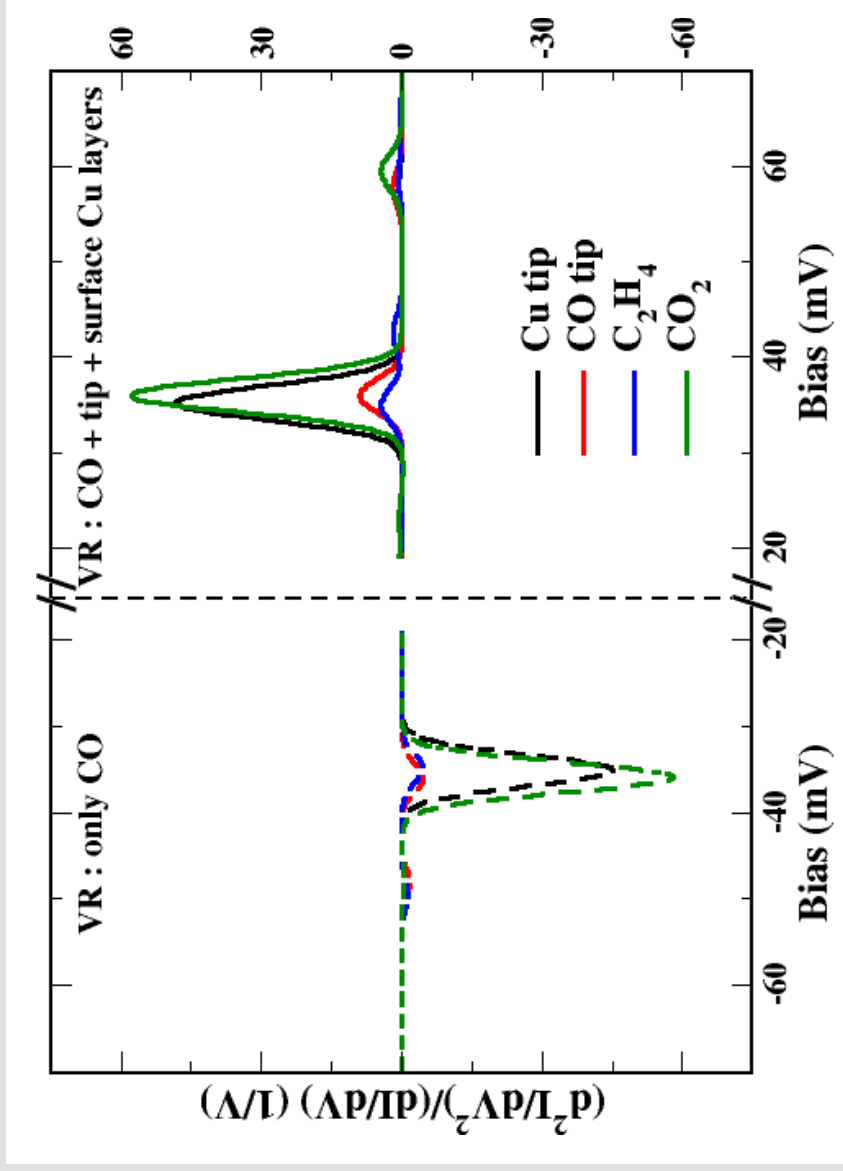


Flat Cu tip



- ✓ Enhancement of CM signal
- ✓ When both CO vibrate: signal from frustrated rotation (FR) is larger than with frozen tip by a factor of ~ 2
- ✓ Flat Cu surface: smaller FR signal. Agreement with experiments. J.R. Hahn and W. Ho, Phys. Rev. Lett. **87**, 196102 (2001)

IETS with different STM tips

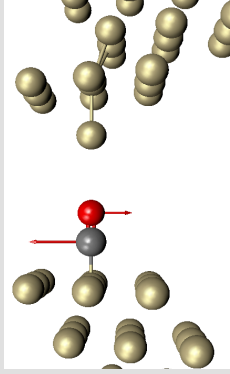
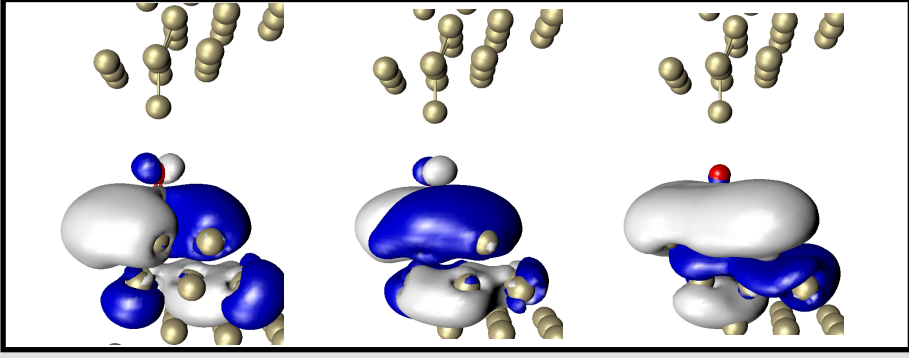


- IETS spectra dominated by FR modes
- FR signal strongly reduced with C_2H_4 tip, in agreement with previous experiments J.R. Hahn and W. Ho, Phys. Rev. Lett. **87**, 196102 (2001)
- Strength of FR signal depends on STM tip

Eigenchannels

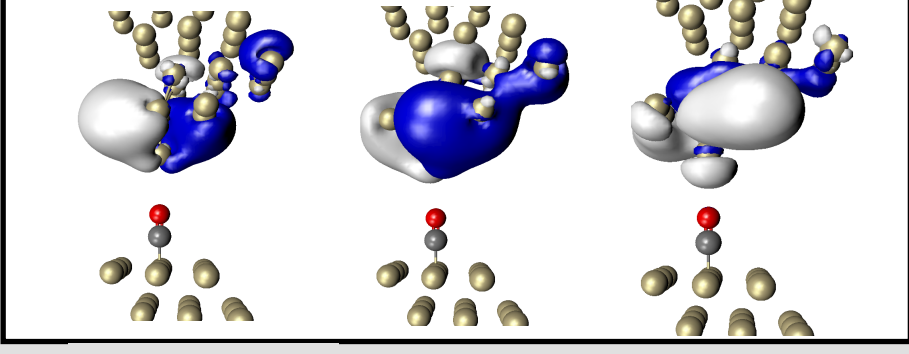


Substrate: CO/Cu(111)



FR

Tip: Cu adatom tip

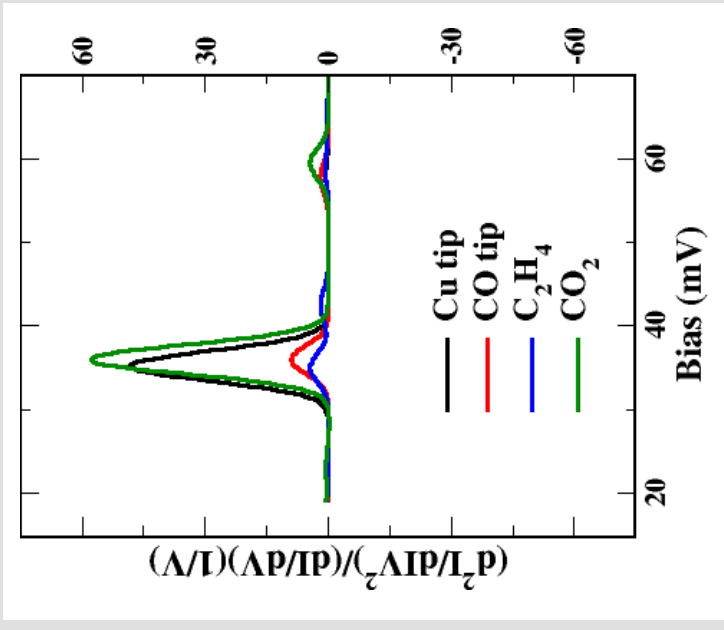
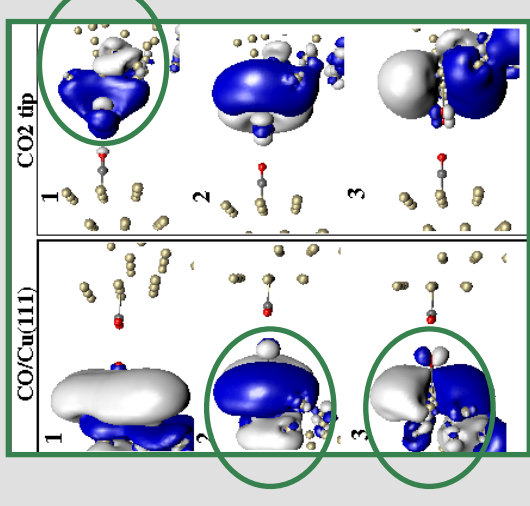
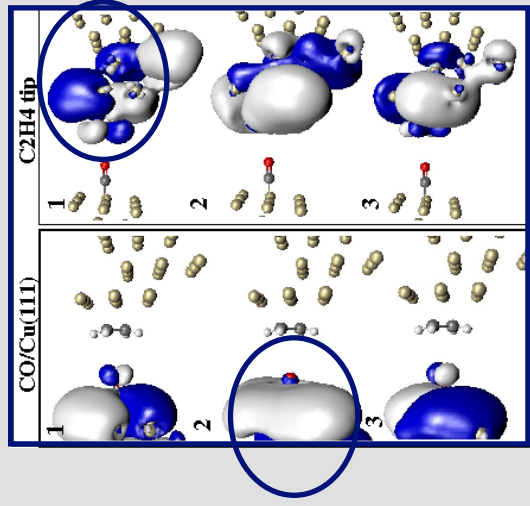
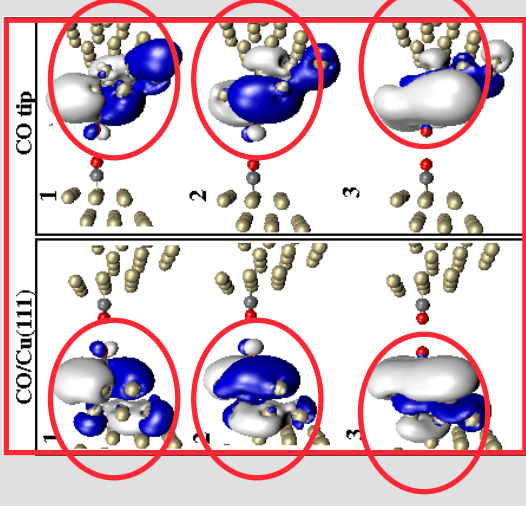
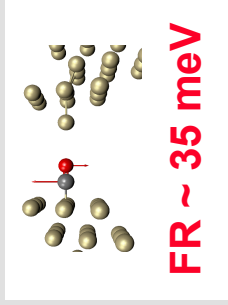
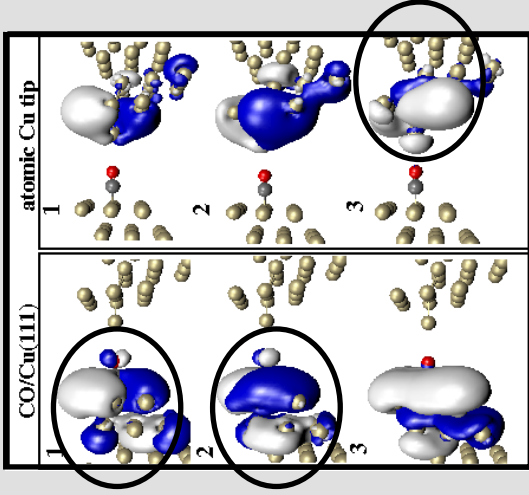


$$\gamma_{FR} = \frac{4\pi e}{\hbar} \sum_{S,T} \left| \langle \psi_S | M_{FR} | \psi_T \rangle \right|^2$$

Inelastic Scattering Rate

M. Paulsson and M. Brandbyge, Phys. Rev. B **76**, 115117 (2007)

Selection rules



Phys. Rev. B 83, 155417(2011)

Conclusions



- Investigation of the role of STM tip on IETS spectra
- Functionalized tips can increase resolving power of IETS and can yield inelastic signals not observed with a metallic tip.
- Modulation of single-molecule IETS via electrode orbital symmetry engineering
- What happens when tip and sample are misaligned?

[Physical Review B 83, 155417\(2011\)](#)
