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Electron transport through single endohedral $Ce@C_{82}$ metallofullerenes

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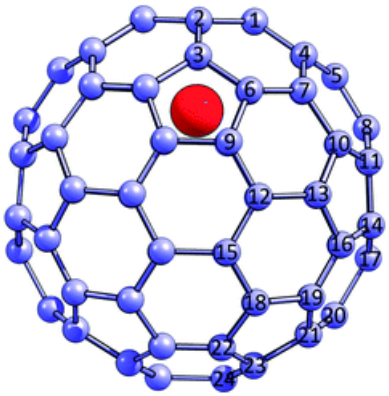
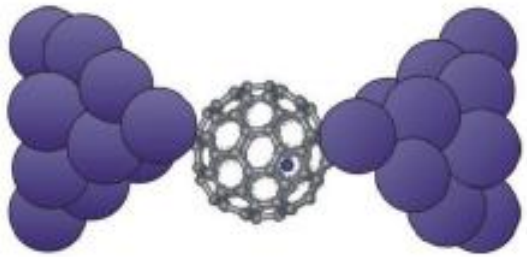




Balogh Zoltán

Nanophysics seminar
Journal Club 2012. october 11.

Kísérleti technika:

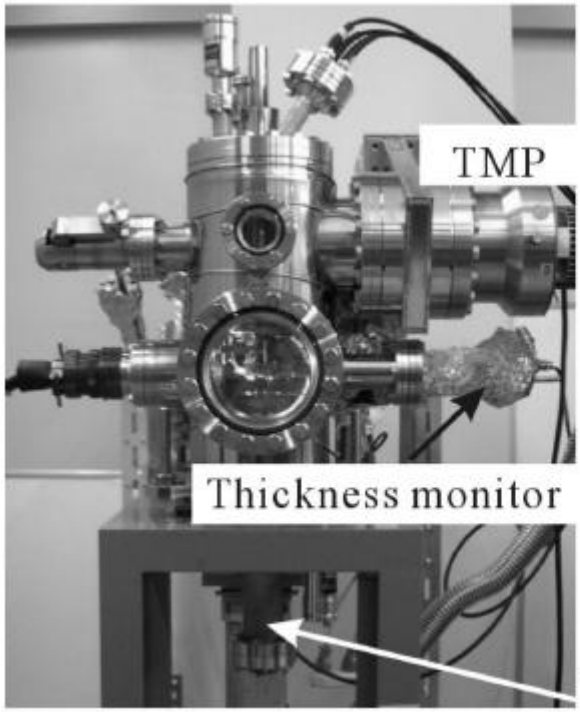
300K-es mérések UHV-ben (2E-7Pa, azaz 2E-9mbar), ugyanolyan MCBJ technikával mint nálunk

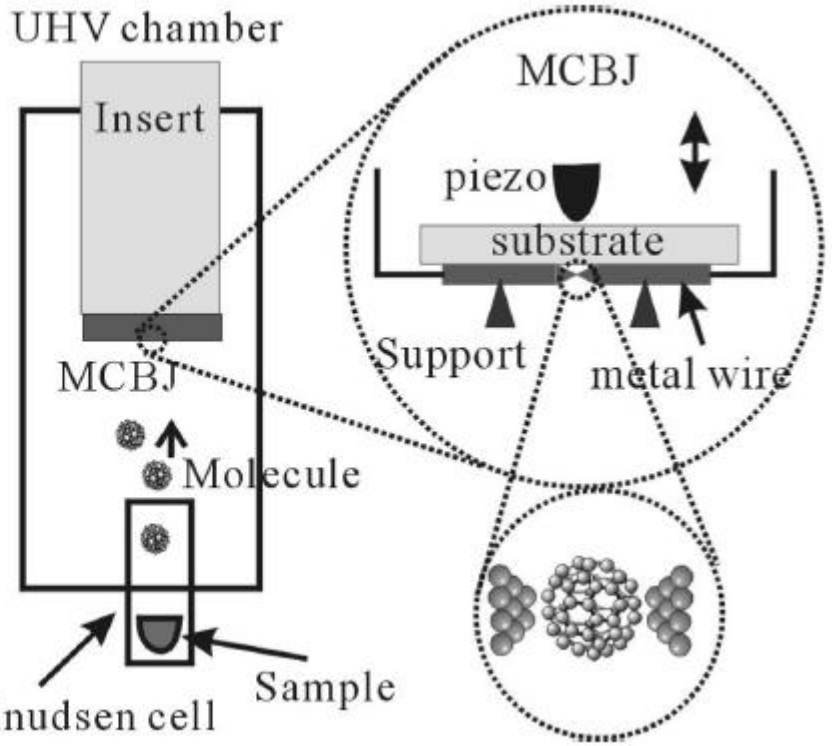
Korábbi tapasztalatok: molekula bejuttatás

oldatban

eltérő viselkedés: pl. stabilitás

UHV (Knudsen cella) nyomás 5E-6Pa (5E-8mbar) alatt





Bevált technika: fullerén és módosulatainak méréséhez

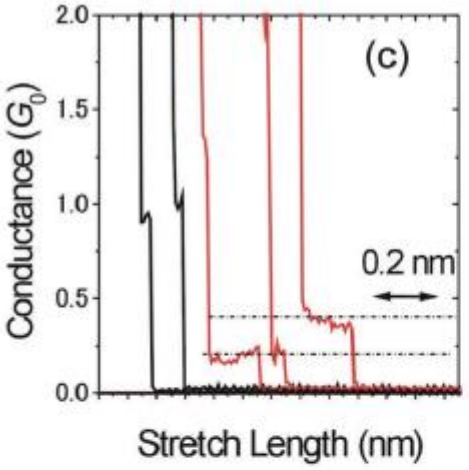
Mérések:

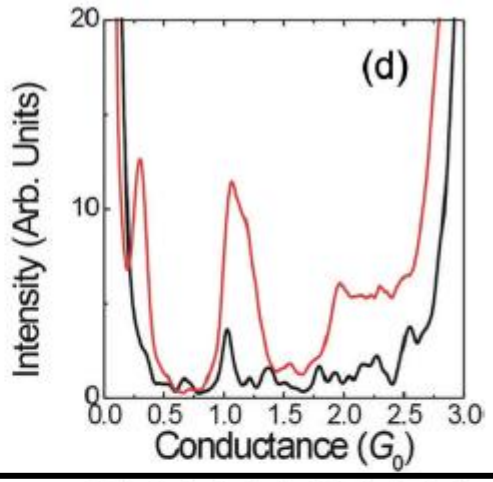
Au és Ag mintákon Ce@C82 molekulákkal és korábbi mérések referenciaként C60 (fullerén) molekulával

Ag-CeC82

0.28G0 ami kisebb mint C60-ra

Elektronok lokalizálódása C82 „ketrecben”



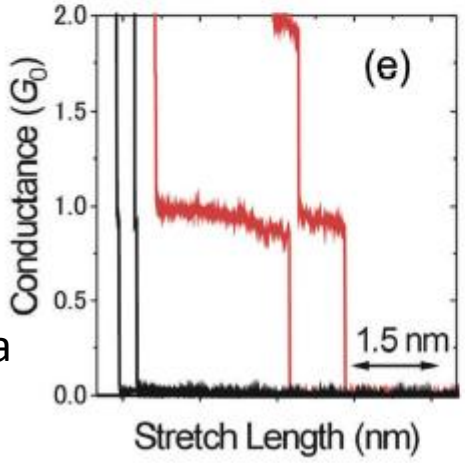


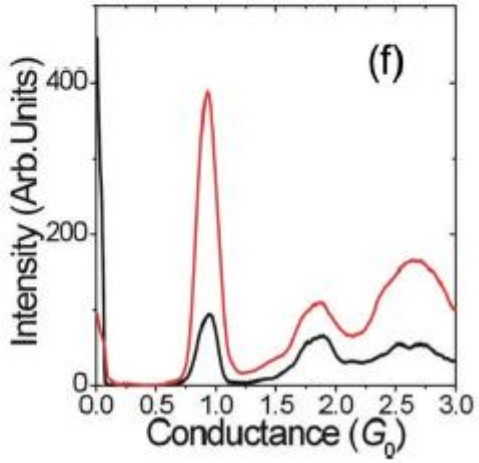
1 vagy 2 molekula beépülése az Ag nanogap-be

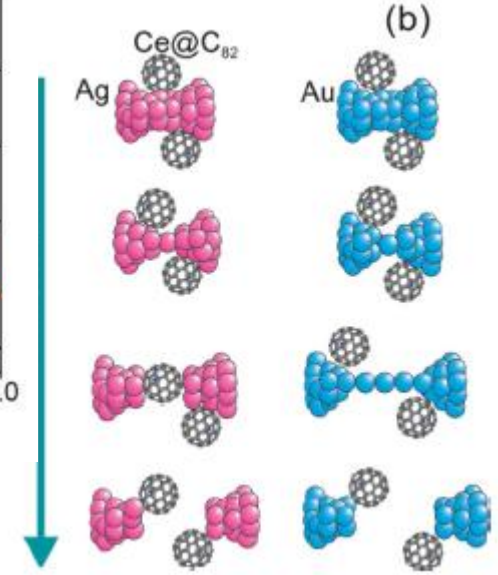
Pi-konjugált Ce@C82 direkt kötése az elektródákhoz

Au

Nem láttak molekulára jellemző platót,
DE 1G0-nál hosszú plató jelent meg és a hisztogram csúcs ennek megfelelően jelentősen nőtt

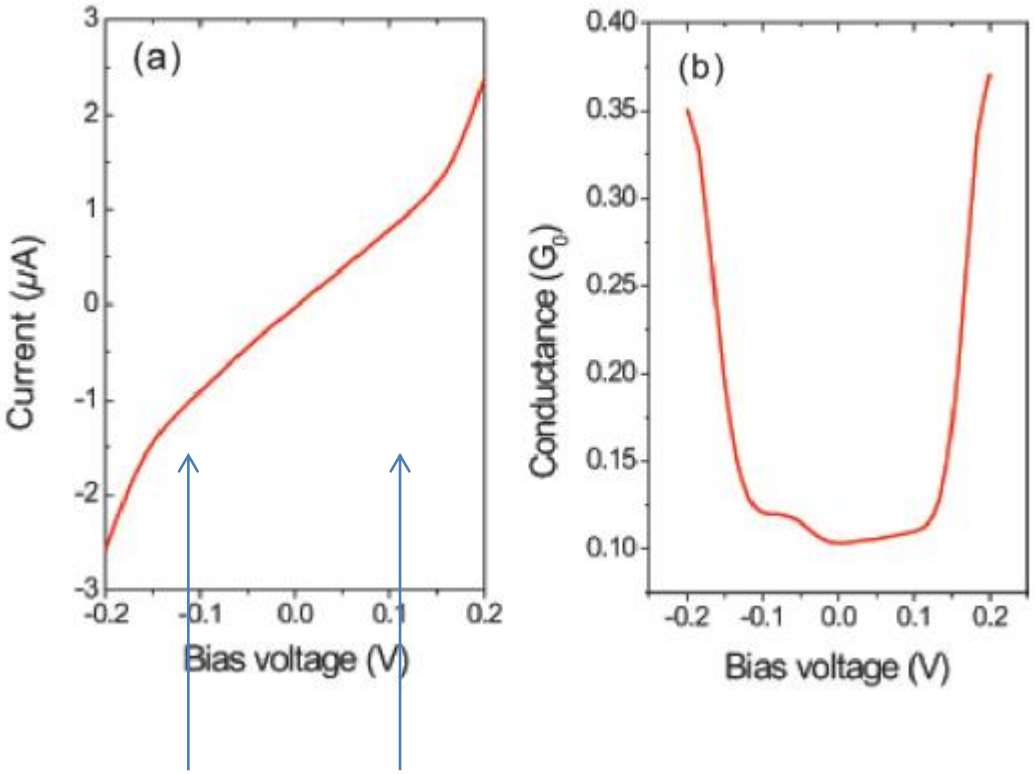






Ag-Ce@C82-Ag kontaktus:

300K-en fix elektródatávolság mellett dc áram-feszültség mérés



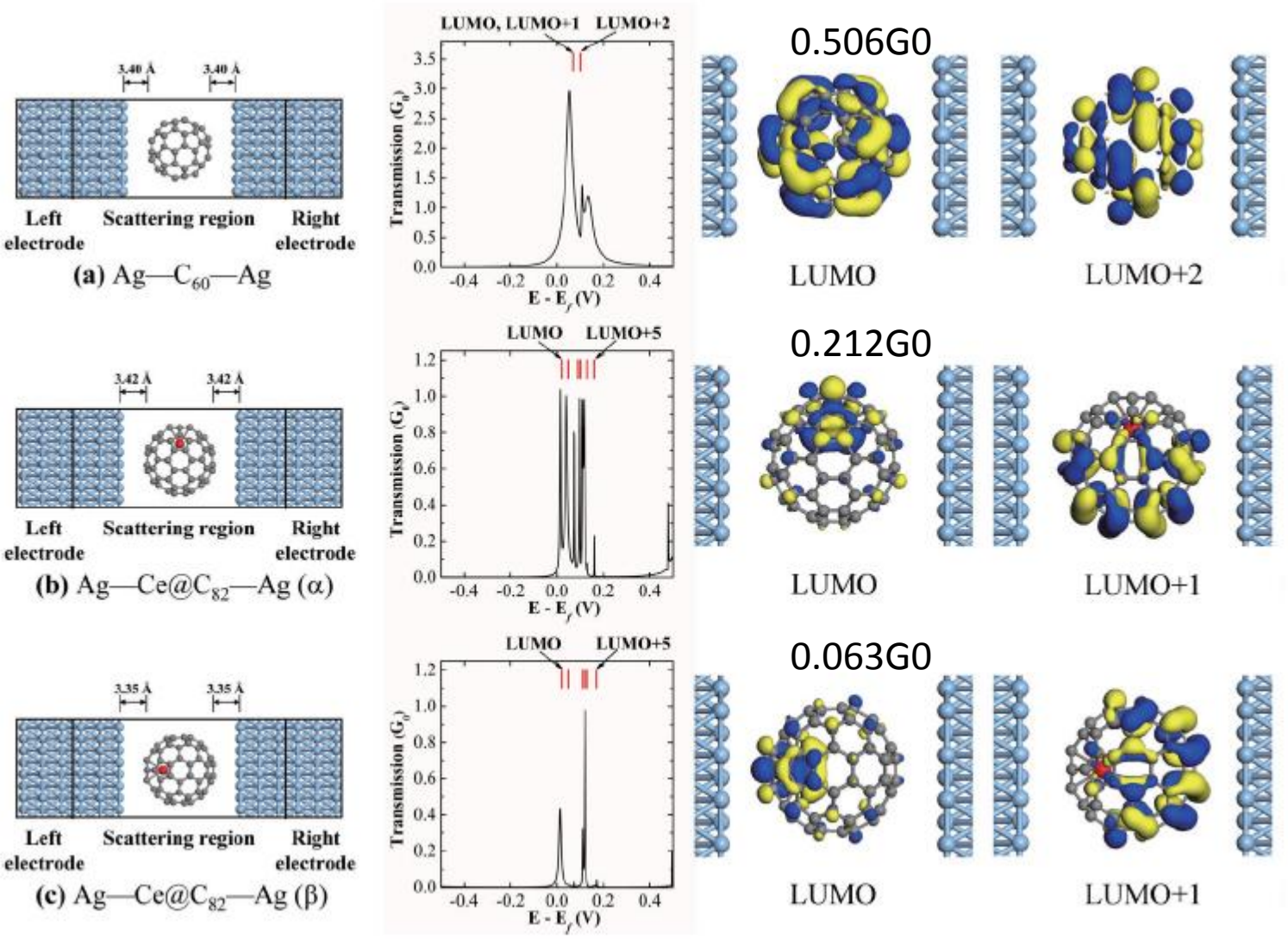
Meredekség váltás 120mV körül

Kis energia gap a HOMO és az elektróda Fermi-szintje között -> megnő a vezetőképesség

DE: Ce atom hatására kisebb HOMO-LUMO gap, egyszerű modellben nagyobb vezetőképességet kellene mutasson

DFT számolások:

Kötési energia (~1.2eV) -> gyenge kötés az elektródákhoz



Számolások és a kísérleti eredmények egyezést mutatnak

Electric Conductance of Single Ethylene and Acetylene Molecules Bridging between Pt Electrodes

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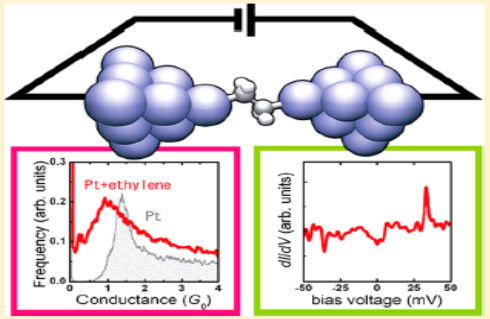
Supporting Information

UHV, 10K

ABSTRACT: We have investigated the conductance and atomic structure of single ethylene and acetylene molecule junctions on the basis of the conductance measurement and vibration spectroscopy of the single molecule junction. Single molecule junctions have a conductance comparable to that of metal atomic junctions (around $0.9G_0$: $G_0 = 2e^2/h$) due to effective hybridization between metal and the π molecular orbital. The ethylene molecules are bound to Pt electrodes via a di-σ bond, while the acetylene molecules are bound to Pt electrodes via di-σ and π bonds. By using the highly conductive single molecule junctions, we investigated the characteristics of vibration spectroscopy of the single molecule junction in an intermediate regime between tunneling and contact. The vibration modes that could modify the conduction orbital were excited for the ethylene and acetylene molecule junctions. The crossover between conductance enhancement and suppression was observed for the single ethylene molecule junction, whereas clear crossover was not observed for the acetylene molecule junction, reflecting the number of conduction orbitals in the single molecule junction.



Metal atomic contact under electrochemical potential control

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Abstract
Electric conductance of the metal atomic contacts of Au and Pd was investigated using a scanning tunneling microscope (STM) in solution under electrochemical potential control. At the hydrogen evolution potential, a fractional conductance peak appeared around 0.5 G_0 ($G_0 = 2e^2/h$) in the conductance histograms of Au contacts. For Pd contacts, peaks appeared around 1.0 G_0 in the conductance histograms at the hydrogen evolution potential. The conductance behavior and atomic configuration of the metal atomic contacts at hydrogen evolution potential were discussed based on previously reported experimental results and theoretical calculation results. We have proposed the formation of hydrogen adsorbed metal Au and Pd contacts in solution at the hydrogen evolution potential.

Electron transport through single π-conjugated molecules bridging between metal electrodes.

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Abstract

Understanding electron transport through a single molecule bridging between metal electrodes is a central issue in the field of molecular electronics. This review covers the fabrication and electron-transport properties of single π-conjugated molecule junctions, which include benzene, fullerene, and π-stacked molecules. The metal/molecule interface plays a decisive role in determining the stability and conductivity of single-molecule junctions. The effect of the metal-molecule contact on the conductance of the single π-conjugated molecule junction is reviewed. The characterization of the single benzene molecule junction is also discussed using inelastic electron tunneling spectroscopy and shot noise. Finally, electron transport through the π-stacked system using π-stacked aromatic molecules enclosed within self-assembled coordination cages is reviewed. The electron transport in the π-stacked systems is found to be efficient at the single-molecule level, thus providing insight into the design of conductive materials.

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Effect of metal-molecule contact on electron-vibration interaction in single hydrogen molecule junction

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The effect of the strength of metal-molecule contact on electron-vibration interaction was investigated for the single hydrogen molecule bridging between Cu electrodes and Pt electrodes. For the single hydrogen/Pt junctions, conductance suppression caused by electron-vibration interaction was observed only for the junction with a conductance value above 0.5 $G_0(G_0 = 2e^2/h)$, which corresponded with the prediction of the one-level model in the symmetric coupling of the molecule to metal electrodes. In contrast, conductance suppression was also observed for the single hydrogen/Cu junctions with a conductance value below 0.5 G_0, which could be explained by a decrease in the interaction between the hydrogen molecule and the Cu electrodes.