Supplementary Information

Structure modulated charge transfer in carbon atomic wires

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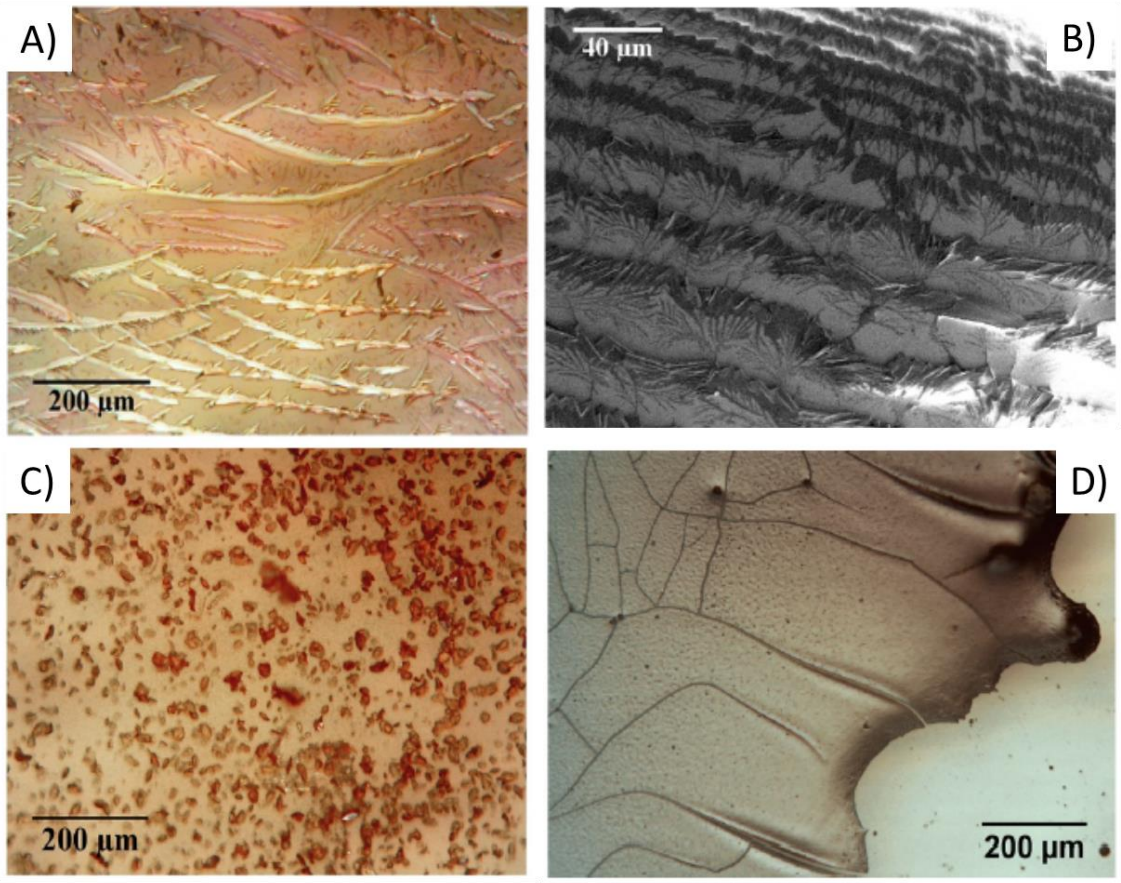

Figure S1: A, B) optical microscopy and SEM image of C2 deposits; C) optical microscopy image of C8; and D) optical microscopy image of C6/TCBD.

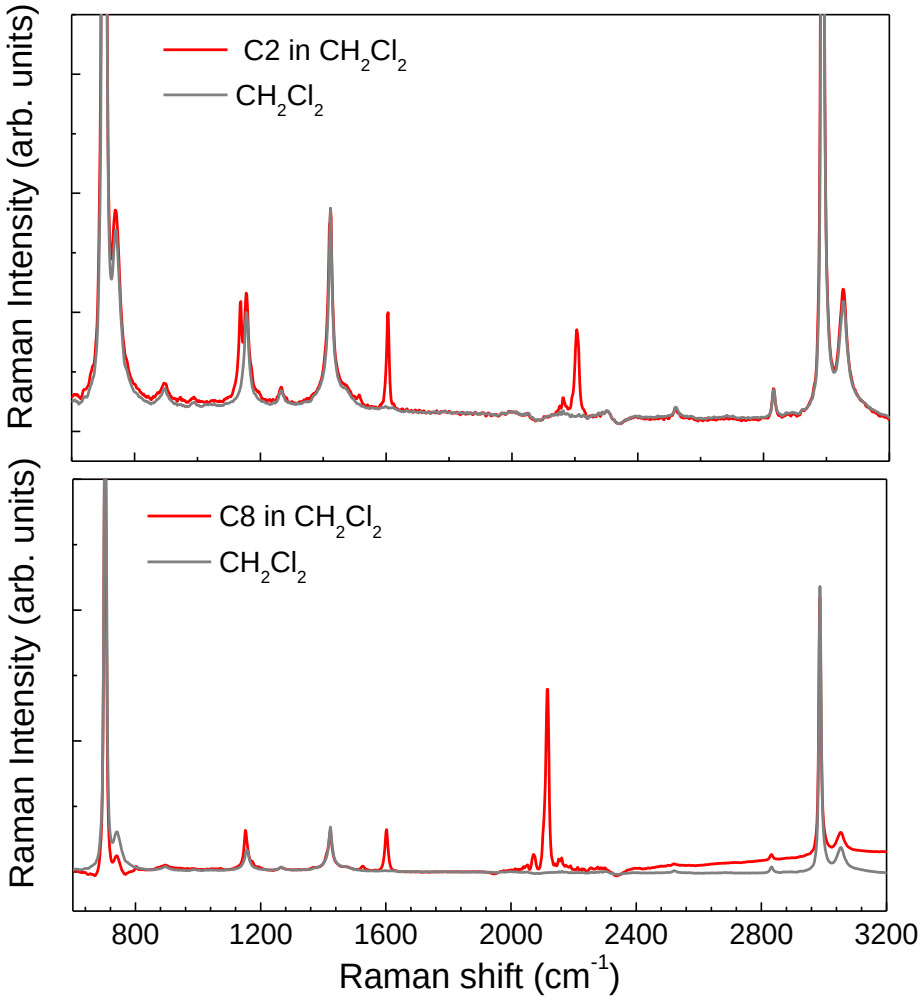

Figure S2: FT-Raman spectra (1064 nm) of C2 and C8 in solution (CH_2Cl_2). The solvent contribution is depicted in grey for comparison.

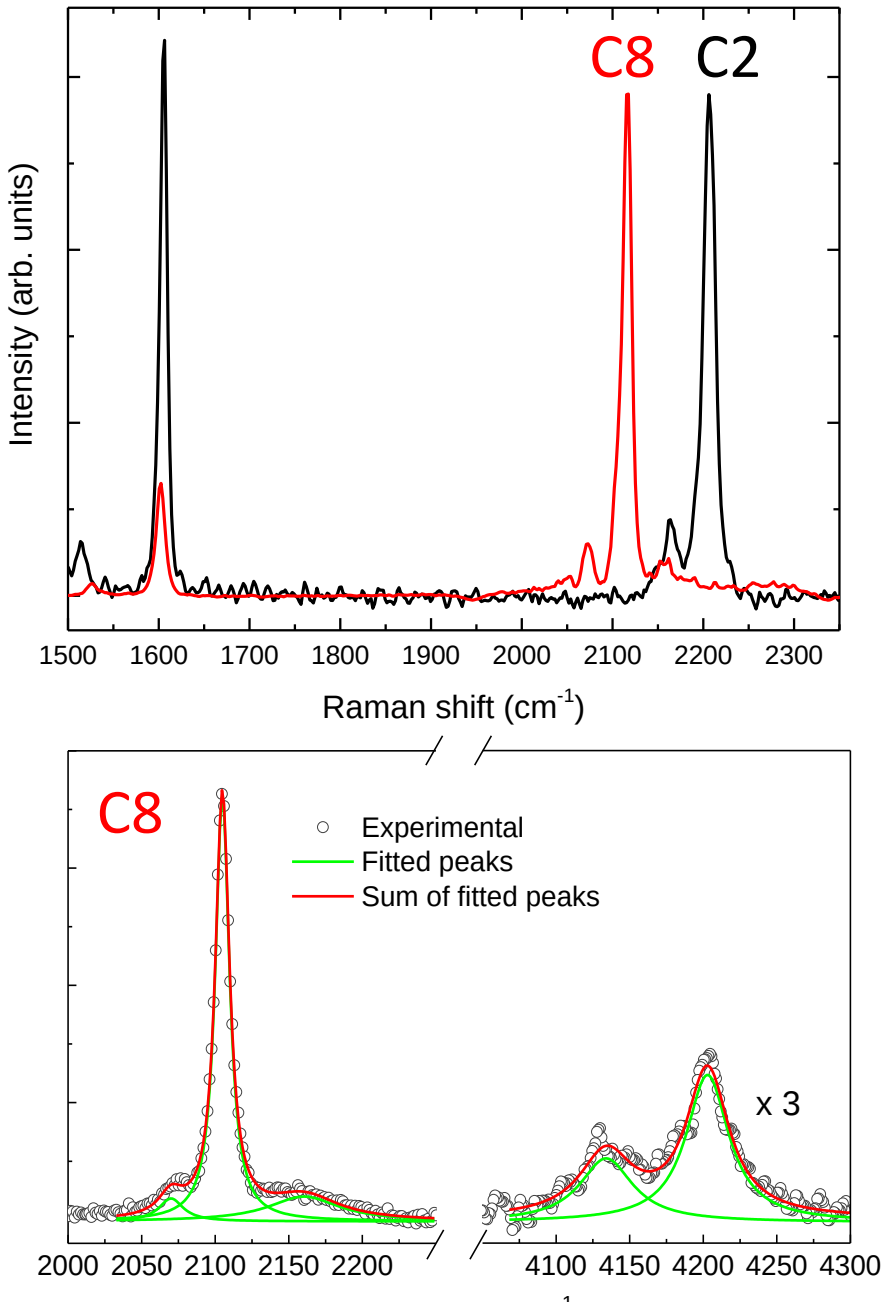

Figure S3: (Top) comparison of FT-Raman spectra of C2 and C8 in solution (CH_2Cl_2; 1064 nm). The contribution of the solvent has been subtracted. (Bottom) fit of ECC mode and second order Raman region for C8.

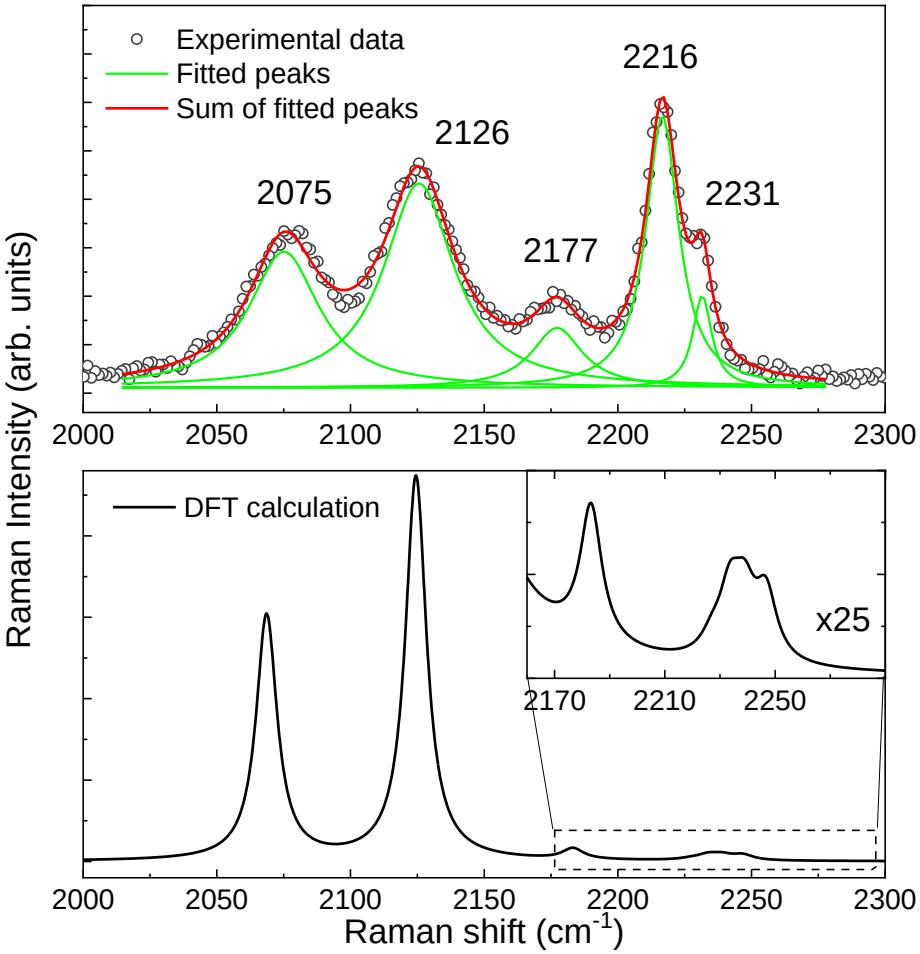

Figure S4: (Top) sp-carbon region detail of the experimental FT-Raman spectrum of C6/TCBD (1064 nm, in film) and fit of the contribution. (Bottom) DFT calculation of the same region.

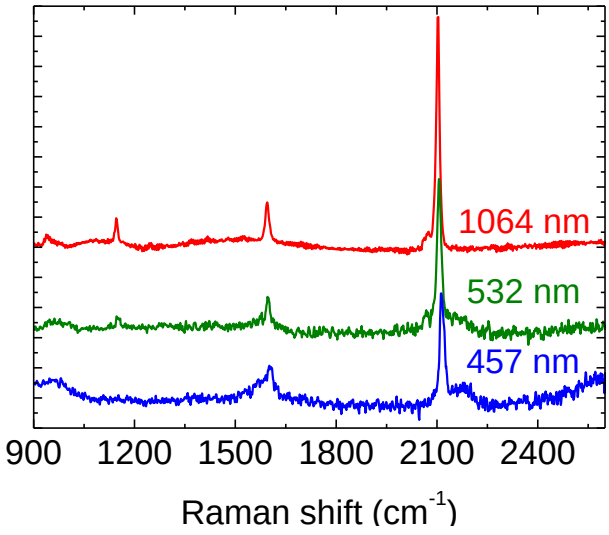

Figure S5: Raman spectra at different wavelengths of C8 deposited in film.

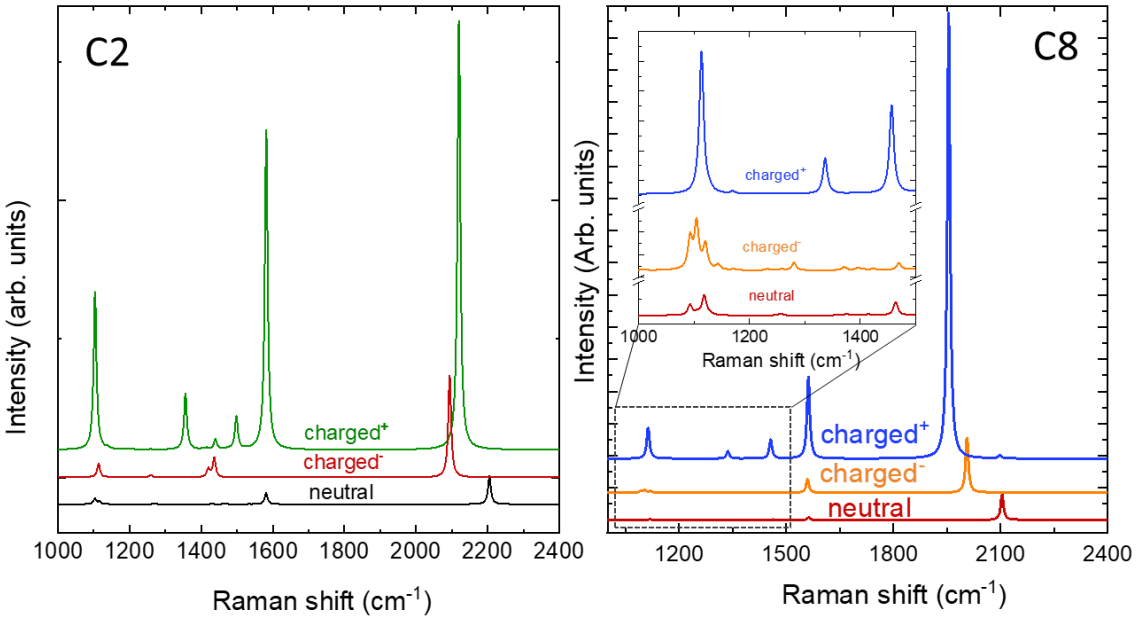

Figure S6: Comparison of DFT computed Raman spectra of neutral, positively and negatively charged C2 (left) and C8 (right) molecule. Details of the region at low frequency (1000-1500 cm^{-1}) is reported in the inset.

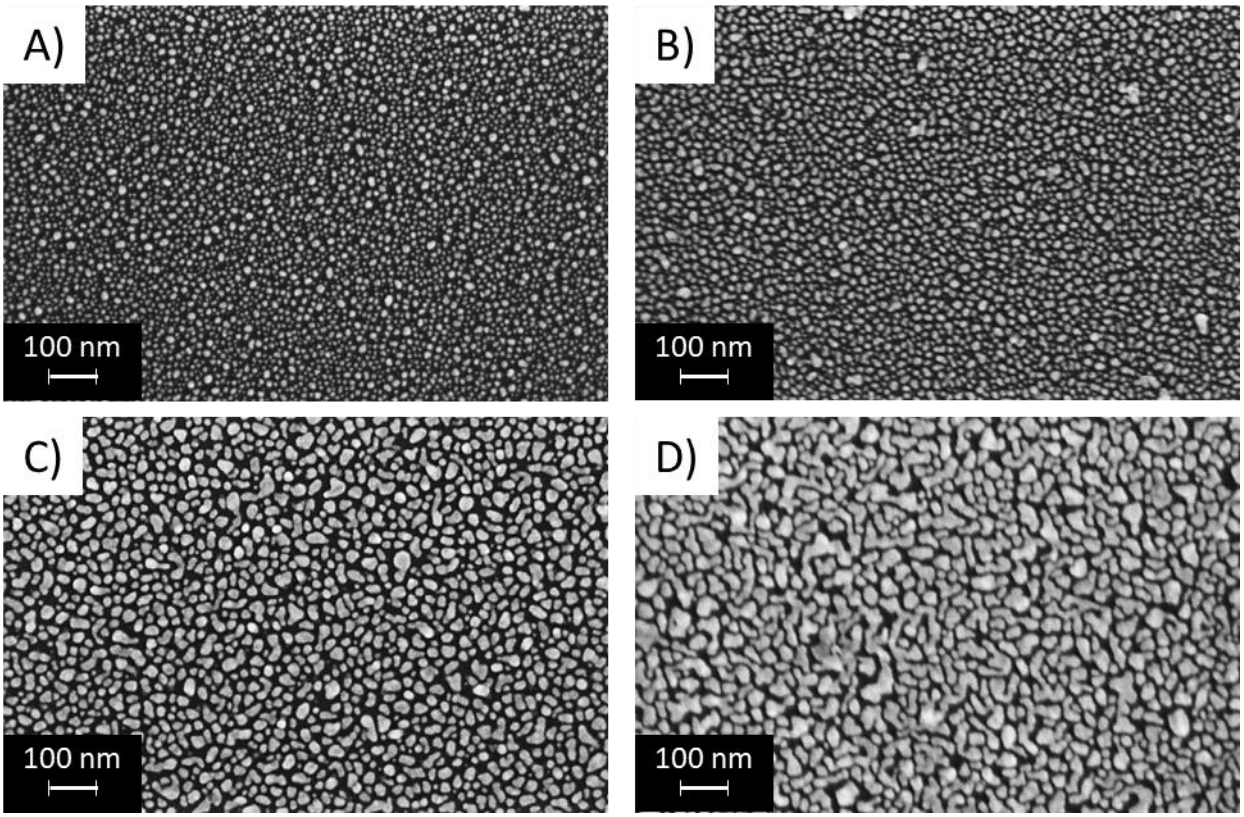

Figure S7: Morphological SEM images of solid SERS-active substrates obtained by vacuum deposition of silver nanoislands.

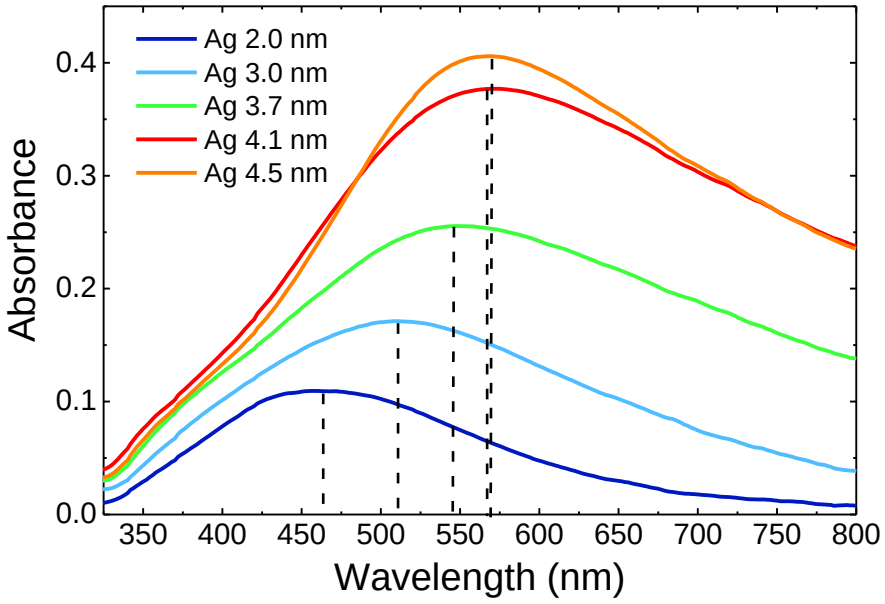

Figure S8: UV-vis absorption spectra of Ag SERS active substrates on glass.

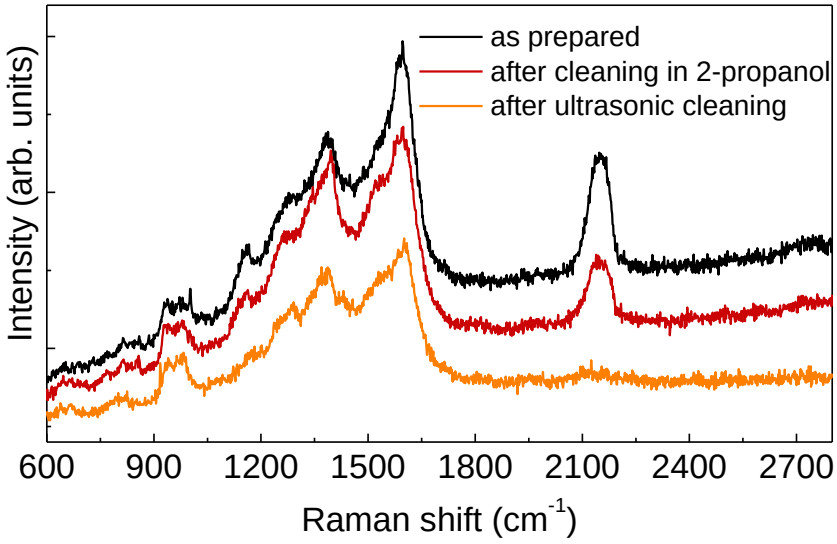

Figure S9: Raman spectra of bare SERS-active substrates (3.0 nm Ag equivalent thickness) as prepared and after different cleaning procedures.

Table S1: DFT computed values of E_{ion} in eV computed for the investigated systems in the two configurations Ag^+/CAW^-, Ag^-/CAW^+; $\Delta E_{ion} = E_{ion}(Ag^+/CAW^-) - E_{ion}(Ag^-/CAW^+)$ is also reported. The values of the BLA (bond length alternation) are reported for neutral and charged systems.

Molecule	Ag^+/CAW^- [eV]	Ag^-/CAW^+ [eV]	ΔE_{ion} [eV]	BLA-neutral [Å]	BLA-charged [Å]
C2	4.329	4.028	+0.301	-	-
C4	3.898	4.031	–0.133	0.1424	0.0973
C6	3.522	4.040	–0.518	0.1323	0.0888
C8	3.050	4.051	–1.001	0.1257	0.0842
C6/TCBD	1.840	5.559	–3.719	0.1167	0.1220