Electronic Supplementary Material (ESI) for Nanoscale.

Supporting Information:

Scanning tunneling microscopy and Raman spectroscopy of polymeric sp–sp^2 carbon atomic wires synthesized on the Au(111) surface

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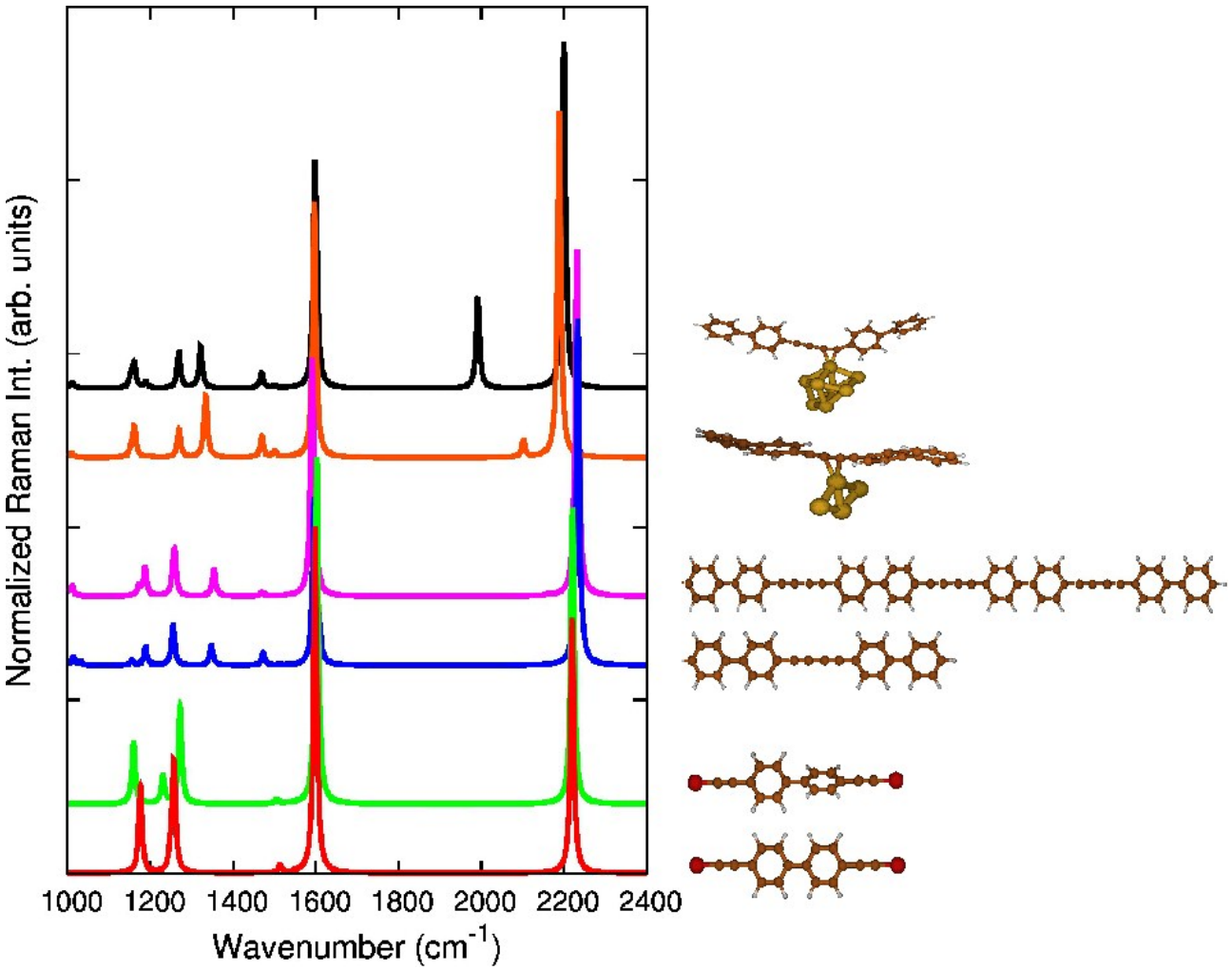

Figure SI1: DFT computed (PBE0/cc-pVTZ, ECP60MDF for Au) Raman spectra of: bBEPB molecular precursor in planar (red) or distorted conformation (green); dimer (blue) and tetramer (purple) molecular models; models of the polymer interacting with Au clusters of different size (Au_4, orange and Au_8, black). The Raman intensities have been normalized to 1 for each model while wavenumbers have been scaled by a factor of 0.96, as explained in the computational details of the paper.

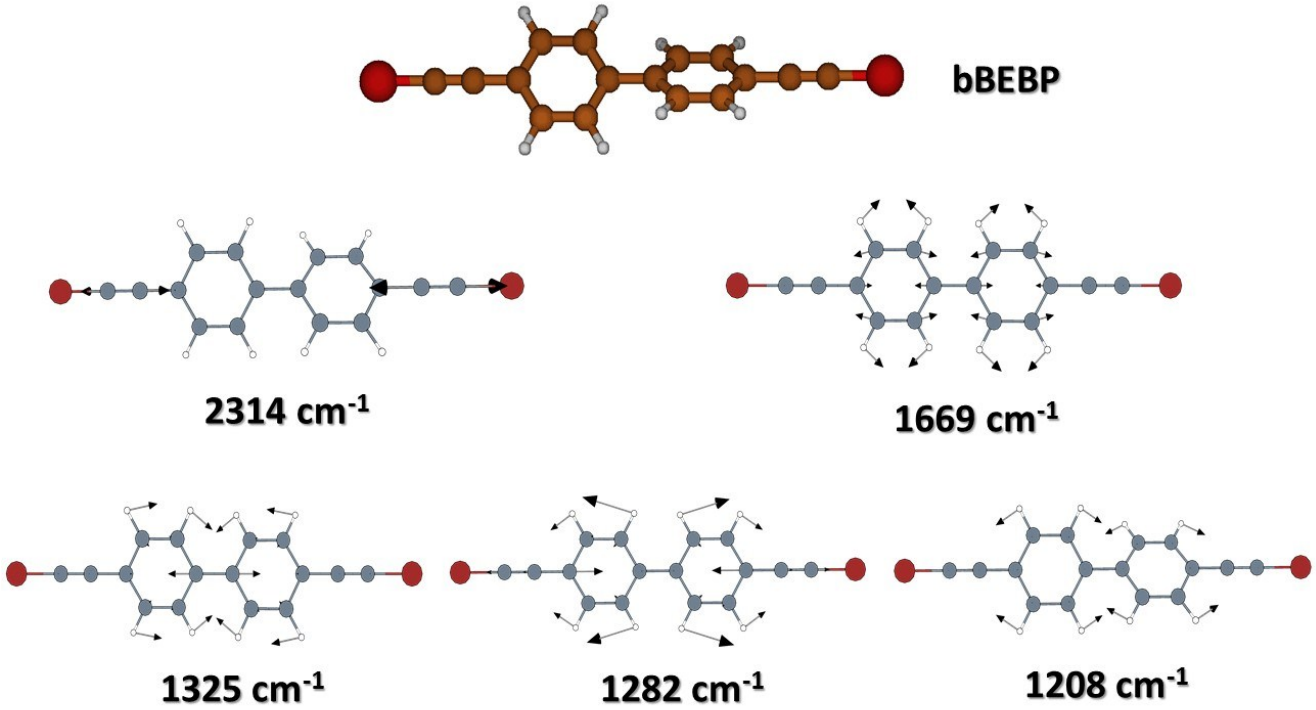

Figure SI2: Sketches of the DFT computed (PBE0/cc-pVTZ) normal modes of vibration associated to the most significant Raman bands of bBEPB molecular precursor (in the distorted conformation), as discussed in the paper. The values of wavenumbers here indicated are unscaled.