Electronic Supplementary Material (ESI) for RSC Advances.

SUPPORTING INFORMATION

Aromatic molecular junctions between graphene sheets: a Molecular Dynamics screening for thermal conductance enhancement.

Alessandro Di Pierro [a], Maria Mar Bernal [a], Diego Martinez [a], Bohayra Mortazavi [b], Guido Saracco [a], Alberto Fina [a,*]

a- Dipartimento di Scienza Applicata e Tecnologia, Politecnico di Torino, Alessandria Campus, Viale Teresa Michel 5, 15121 Alessandria, Italy

b- Institute of Structural Mechanics, Bauhaus-Universität Weimar Marienstraße. 15, D-99423 Weimar, Germany

1. Thermal simulations

Figure S1 shows to the energy flowing through thermostats during simulations, for selected junctions, taken as examples. All other junction exhibited similar linear plots. Positive slopes refers to energy provided to the system while negative slopes refers to the subtracted one. A symmetrical trend, for the same molecule, indicates almost no gain or loss of energy during runtime. The slope calculation also provides the heat flux values needed to evaluate thermal conductance in Fourier's law.

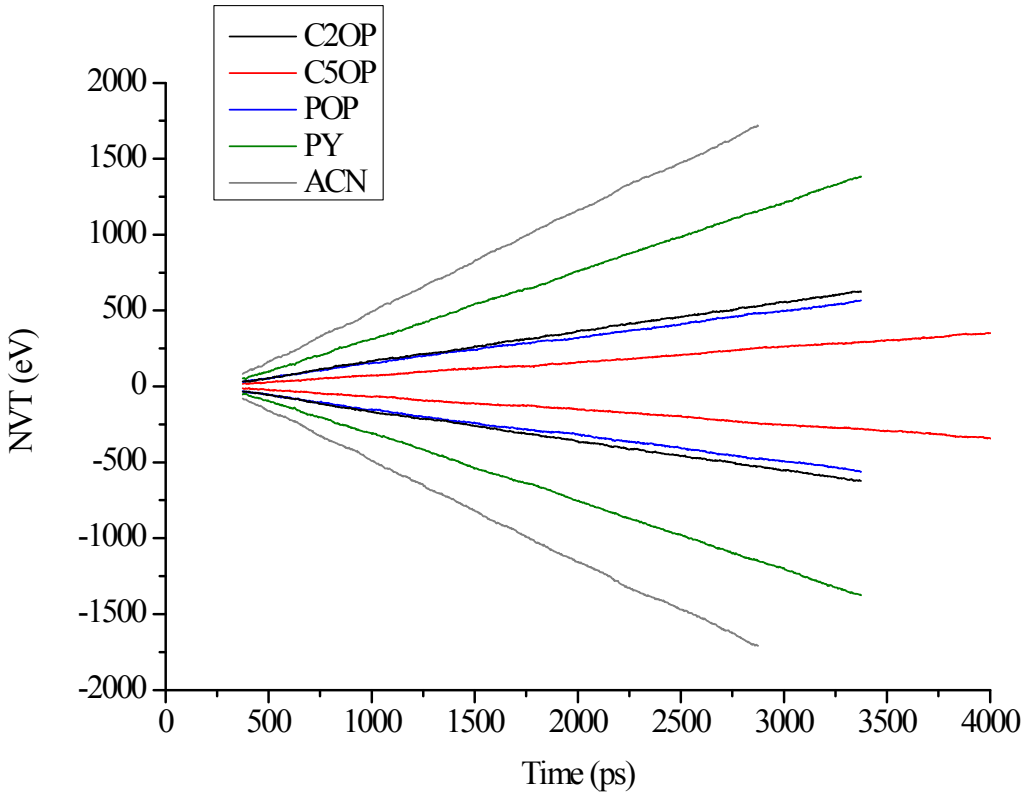

Figure S1: Energy versus time plot for selected molecules taken as example.

To calculate TBC, the temperature profile was calculated by slicing the models along x coordinate: the temperature plots for selected junction are provided in Figure S2. The temperature of the thermal jump was evaluated from the projection of the slopes in the center of the junction. The reported temperature profiles are similar for all models, with higher slopes and lower thermal jumps were recorded for higher conductive models.

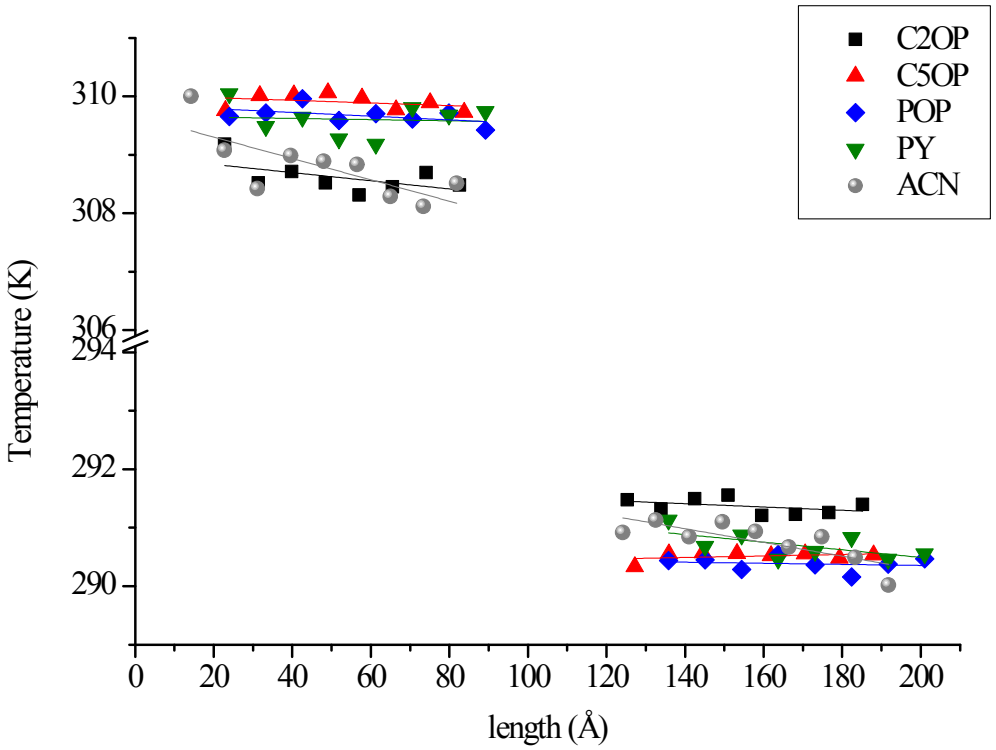

Figure S2: Temperature profile across different molecular junctions, taken as example. For clarity, a temperature break is introduced in 294-306 K range.

2. Tensile simulations

The simulation box included six copies of the model over z-axis. Stress strain data were averaged to improve accuracy. Figure S3 reports the initial linear stage, form 0 up to 10%, in tensile testing for all the molecules discussed. The linear fitting of those curves provided the elastic modulus of the junctions. The molecular volume[1, 2] considered for the calculation of the tensile modulus was taken as half of the volume among the edges interface (in x,y,z of about d*5*3.4 $Å^3$). To replicate the results by changing the velocity seed, the tensile modulus exhibited a variation less than of one percent.

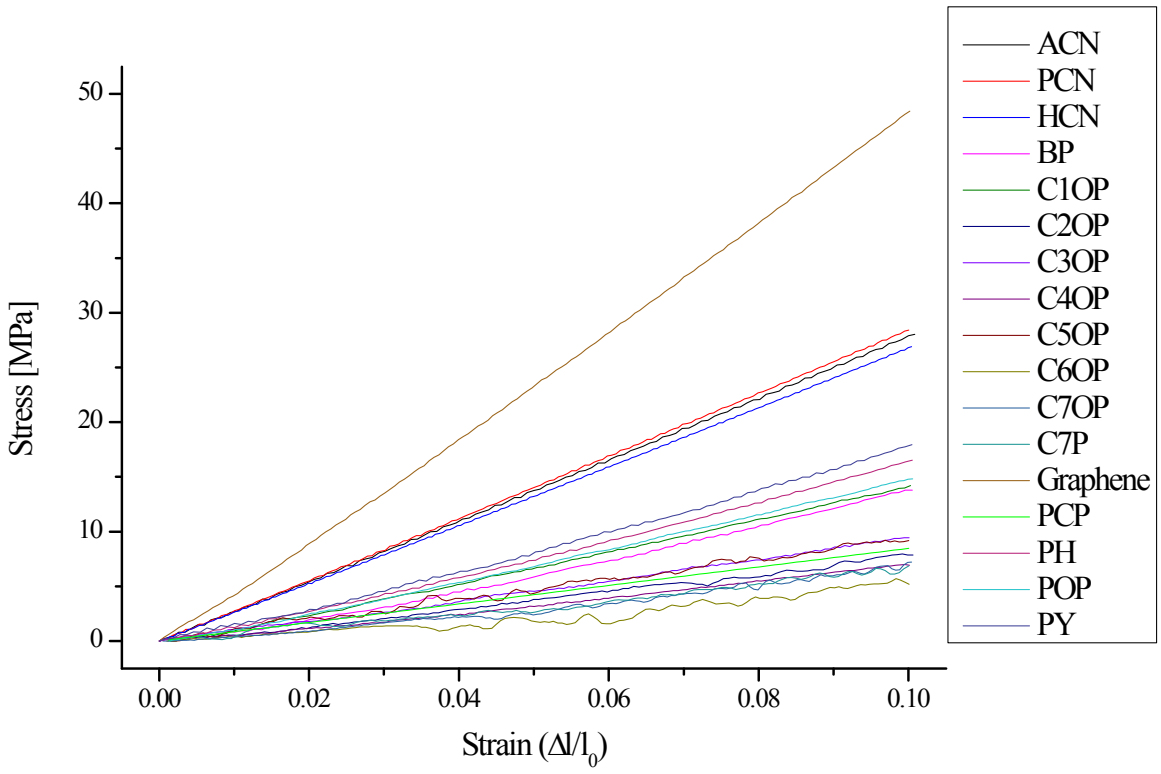

Figure S3. Calculated stress-strain plots from MD simulations, small nonlinearities are due to molecular rearrangements.

3. Force Field parameters

In this work, the bond stiffness, depends on the COMPASS[3] force field parameters. Figure S4 represents briefly the atom types contained in various molecular junctions. Table S1 contains Bond coefficients for ether oxygen, aromatic and alkyl carbon relevant to tensile simulations.

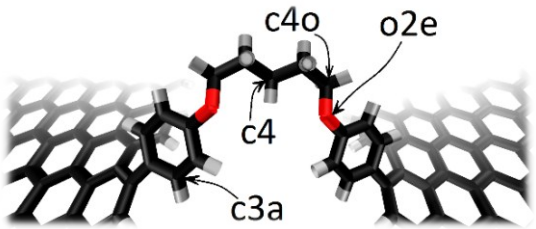

Figure S4: COMPASS© Atom types for oxygen and carbon adopted in C5OP molecular junction taken as example.

Table S1: Bond coefficients for ether oxygen (o2e), aromatic (c3a) and alkyl carbon (c4) adopted in COMPASS force field.

$E = K_2(r - r_0)^2 + K_3(r - r_0)^3 + K_4(r - r_0)^4$	**r_0**	**K2**	**K3**	**K4**
o2e-c3a	1.37	428.88	-738.23	1114.96
o2e-c4o	1.42	400.39	-835.19	1313.01
c4o-c4	1.53	299.67	-501.77	679.81
c4-c4	1.53	299.67	-501.77	679.81

References

[1] A.P. Thompson, S.J. Plimpton, W. Mattson, General formulation of pressure and stress tensor for arbitrary many-body interaction potentials under periodic boundary conditions, The Journal of chemical physics 131(15) (2009) 154107.

[2] D.M. Heyes, Pressure tensor of partial-charge and point-dipole lattices with bulk and surface geometries, Physical Review B 49(2) (1994) 755-764.

[3] H. Sun, COMPASS: An ab Initio Force-Field Optimized for Condensed-Phase ApplicationsOverview with Details on Alkane and Benzene Compounds, The Journal of Physical Chemistry B 102(38) (1998) 7338-7364.