

Supplementary Materials: Electronic and transport properties of two-dimensional conjugated polymer networks including disorder.

1

Jean-Joseph Adjizian,* Aurélien Lherbier, Simon Dubois, Andrés Rafael
Botello-Méndez, and Jean-Christophe Charlier

*Université catholique de Louvain, Institute of Condensed Matter and Nanosciences,
Chemin des étoiles 8, 1348 Louvain-la-neuve, Belgium*

E-mail: jean.adjizian@uclouvain.be

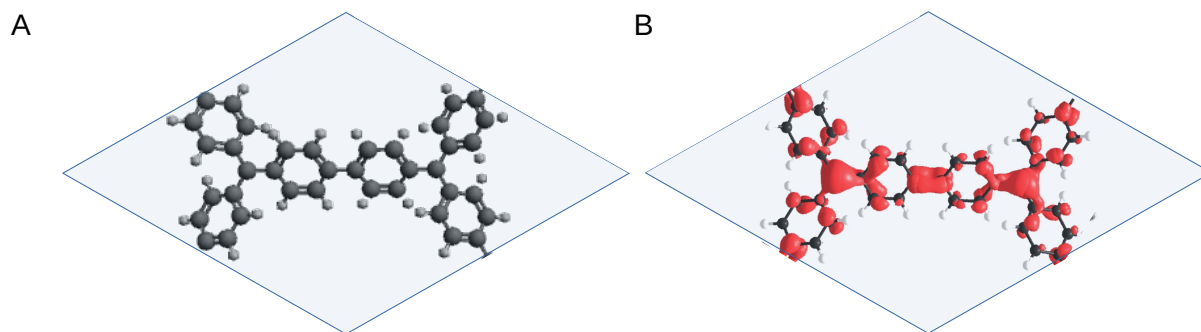


Figure 1: (A) A pristine 2DCP cell and (B) the corresponding wave function at the highest occupied state (at K-point).

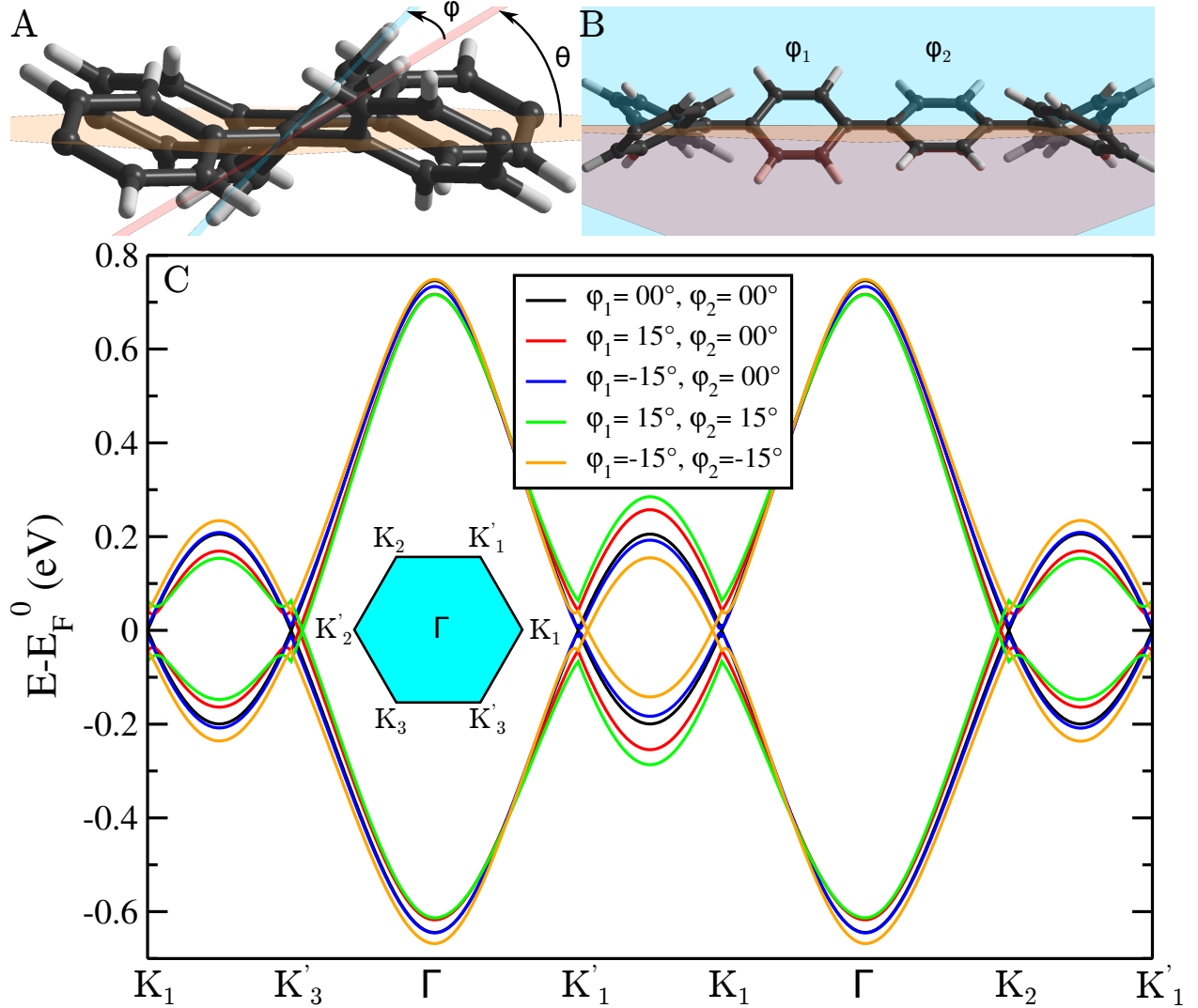


Figure 2: Effect of various benzene rotations on the electronic properties of the 2D conjugated polymer network. (A) Side view along a branch axis of the primitive cell, θ represents the dihedral angle between a branch and the XY plan. φ represents the dihedral angle between benzene rings and θ . (B) Side view perpendicular to the branch axis in (A). φ_1 represents the dihedral angle of the first benzene ring and φ_2 represents the dihedral angle of the second benzene ring with respect to θ . (C) First-principles electronic band structures for structures with different rotational angles. The black curve is the ground state band structure ($\theta=30.8^\circ$ and $\varphi_1=\varphi_2=0^\circ$), the red and blue curves are the band structures with a single benzene ring rotated by $+15^\circ$ ($\varphi_1=15^\circ, \varphi_2=0^\circ$) and -15° ($\varphi_1=-15^\circ, \varphi_2=0^\circ$) respectively. The green and orange curves are the band structures with a branch rotated by $+15^\circ$ ($\varphi_1=\varphi_2=15^\circ$) and -15° ($\varphi_1=\varphi_2=-15^\circ$).

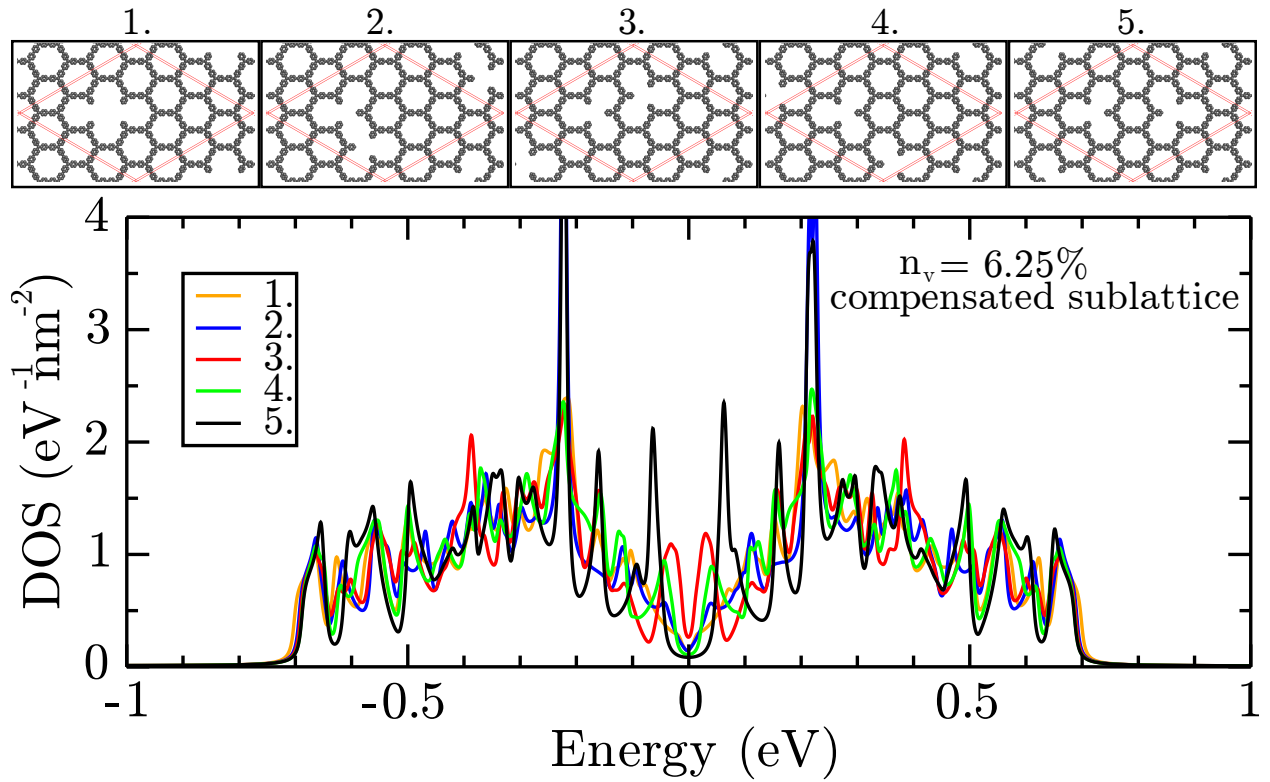


Figure 3: A 4x4 2DCP cell containing 6.25% of vacancies. For each structure, from 1 to 5, there are two vacancies: one located on the sub-lattice "A" and one on the sub-lattice "B". These five different configurations are investigated and their respective DOS are shown.