

Tunable Dirac Cones and Flat Bands in Mesoscale Ordered Two-dimensional Semiconductor Polymers

Giorgio Contini^{a,b}

^a *Istituto di Struttura della Materia-CNR (ISM-CNR), Via Fosso del Cavaliere 100, 00133 Roma, Italy*

^b *Department of Physics, University Tor Vergata, Via della Ricerca Scientifica 1, 00133 Roma, Italy*

Corresponding author email: giorgio.contini@ism.cnr.it

Dirac cones, present in the band structure of graphene, are responsible of its remarkable charge-transport properties. However, they are not exclusive to graphene but require that the material presents specific symmetry and delocalized electrons. Efforts have been devoted to identifying 2D materials beyond graphene that offer a greater degree of tunability and a non-zero band gap while retaining high carrier mobility [1].

On-surface synthesis represents an opportunity to manipulate the electronic band structure of the material by varying the molecular building blocks (e.g. by the change of constituent atoms and symmetry). By using a class of heteroatom substituted triangulene monomers we synthesized mesoscale ordered 2D π -conjugated polymers on Au(111) with semiconducting properties arranged in a kagome lattice showing Dirac cone structures and flat bands [2], theoretically predicted [3]. We demonstrate that it is possible to tune the Dirac cone structures and flat bands energy positions by changing the bridging atoms in the triangulene monomers [4]. These results overcome the major barriers to the application of 2D π -conjugated polymers due small domain size and high defect density attained so far. Although the 2D polymers have been obtained on a metal surface, they can be detached and transferred to other substrates to be used in devices.

References

- [1] K. Asano and C. Hotta, Phys. Rev. B 2011, 83, 245125; J. Wang, S. Deng, Z. Liu and Z. Liu, Natl Sci. Rev. 2015, 2, 22.
- [2] Y. Jing and T. Heine, J. Am. Chem. Soc. 2019, 141, 743.
- [3] G. Galeotti, F. De Marchi, E. Hamzehpoor, O. MacLean, R. M. Rao, Y. Chen, L. V. Besteiro, D. Dettmann, L. Ferrari, F. Frezza, et al., Nature Materials 2020, 19, 874.
- [4] D. Dettmann, P. M. Sheverdyeva, S. Franchi, G. Galeotti, P. Moras, C. Ceccarelli, D.F. Perepichka, F. Rosei and G. Contini, ACS Nano 2024, 18, 849.