CNMS Staff Science Highlight

Surface-Induced Orientation Control of CuPc Molecules for the Epitaxial Growth of Highly Ordered Organic Crystals on Graphene

Scientific Achievement

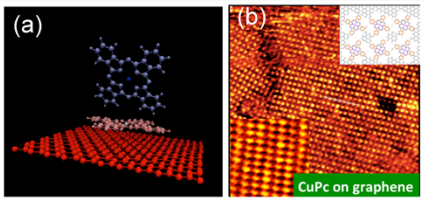
Graphene was shown to direct the assembly of copper phthalocyanine (CuPc) molecules into epitaxially-aligned superstructures relevant to organic electronics. Theoretical modeling of the mechanisms responsible for this alignment revealed that van der Waals interactions and interfacial dipole interactions induced by charge transfer both play important roles.

Significance

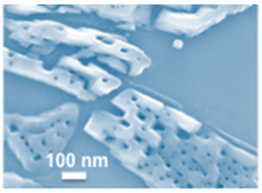
Fundamental understanding of molecular interactions at interfaces is important to control the nanoscale morphology and orientation of organic semiconductors to improve optoelectronic processes for high-performance organic electronic devices. Here, graphene is demonstrated to effectively template CuPc molecules to nucleate, orient, and pack in the face-on orientation, the ideal structure for high-performance organic photovoltaics.

Research Details

- CuPc was thermally evaporated in high vacuum onto both as-grown graphene on Cu, and graphene transferred onto Si substrates.
- The nucleation, orientation and packing of CuPc molecules on films of graphene were investigated in a systematic experimental and theoretical investigation that combined X-ray scattering and diffraction, scanning probe microscopy, and electron microscopy with first-principles calculations.



(a) Theoretical modeling of CuPc molecules interactions with graphene in both face-on and side-on orientations (b) STM image of CuPc molecules aligned in the face-on orientation on graphene. Bottom left inset is a higher magnification STM image, top right inset schematically shows the molecular orientation.



SEM image of large 2D strip-like crystals of CuPc that are epitaxially aligned with the graphene surface and oriented along the graphene grain boundaries.

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Highlight Narrative

The epitaxial growth and preferred molecular orientation of copper phthalocyanine (CuPc) molecules on graphene has been systematically investigated and compared with growth on Si substrates, demonstrating the role of surface-mediated interactions in determining molecular orientation. X-ray scattering and diffraction, scanning tunneling microscopy, scanning electron microscopy, and first-principles theoretical calculations were used to show that the nucleation, orientation and packing of CuPc molecules on films of graphene are fundamentally different compared to those grown on Si substrates. Interfacial dipole interactions induced by charge transfer between CuPc molecules and graphene are shown to epitaxially align the CuPc molecules in a face-on orientation in a series of ordered superstructures. At high temperatures, CuPc molecules lie flat with respect to the graphene substrate to form strip-like CuPc crystals with micron sizes containing monocrystalline grains. Such large epitaxial crystals may potentially enable improvement in the device performance of organic thin films, wherein charge transport, exciton diffusion and dissociation are currently limited by grain size effects and molecular orientation.

Reference:

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