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Self-assembly of functionalized indoles on surfaces FABRIZIO DE MARCHI, DALING CUI, JOSH LIPTON-DUFFIN, Institut National de la Recherche Scientifique, Centre Énergie, Materiaux, Telécommunications, 1650 Lionel Boulet Boulevard, J3X 1S2 Varennes, CLARA SANTATO, Département de Génie Physique, École Polytechnique de Montréal, C.P. 6079, Succ. Centre Ville, H3C 3A7, Canada, JENNIFER MACLEOD, FEDERICO ROSEI, Institut National de la Recherche Scientifique, Centre Énergie, Materiaux, Telécommunications, 1650 Lionel Boulet Boulevard, J3X 1S2 Varennes — To predict how a molecule on a surface will interact with its neighbors or with the substrate itself is an intriguing challenge. If overcome, it would allow the design of a pattern by the proper selection of monomers. However, we are far from a complete understanding of self-assembly mechanisms on surfaces, and more insight can be gathered by studying small, simple systems. In nature, small molecules are the building blocks for more complex systems, such as enzymes and DNA; understanding their self-assembly could lead to the ability to encode this kind of complexity and information density into engineered self-assembled molecular structures. We report here on the self-assembly of two simple molecules: indole 2-carboxylic acid (I2CA) and 5,6-dihydroxyindole-2-carboxylic acid (DHICA) over various substrates. DHICA is one of the monomers that forms eumelanin, and brings the possibility of different bonding architectures due to its combination of carboxyl and hydroxyl groups. At surfaces, DHICA forms a number of structures depending on the conditions used to prepare the molecular film. On the other hand, I2CA self-assembles into a simple ordered pattern that is relatively independent of the substrate and preparation conditions. DFT calculations corroborate these observations.

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