

Abstract Submitted  
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**Coupling between diffusion and orientation of pentacene molecules on an organic surface** BRUNO ECKHARDT, PAUL ROTTER, ANTONIA MORHERR, GREGOR WITTE, Fachbereich Physik, Philipps-Universität Marburg, BARBARA AJ LECHNER, DAVID M CHISNALL, DAVID J WARD, ANDREW P JARDINE, JOHN ELLIS, WILLIAM ALLISON, Cavendish Laboratory, University of Cambridge — We have used Helium Spin Echo (HeSE) to unveil the intricate motion of pentacene ad molecules diffusing on a chemisorbed monolayer of pentacene on Cu(110), a stable, well-ordered organic model surface. HeSE is unique in that it provides access to diffusion on the relevant nm and ps spatial and temporal time scale, respectively, and in not being restricted to low temperatures. The interpretation of the observed scattering data is assisted by Langevin simulations of trajectories on potential energy surfaces extracted from MM3 force fields. We find that the molecules show a strong coupling between the direction of diffusion, the orientation of the adsorbed molecule, and the orientation of the molecules in the monolayer. Specifically, we find that pentacene moves along tracks that are either parallel or perpendicular to the orientation of the molecules on the surface. The molecules are aligned with the direction of motion. The experimental data are explained by ad molecule rotation that enables a switching between diffusion directions. The results extend our understanding of diffusion in complex organic systems on the molecular level and highlight the importance of orientation-diffusion coupling for elongated molecules. Rotter et al, Nature Materials 15:397 (2016)

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