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**Tuning Structural and Mechanical Properties of Two-Dimensional Molecular Crystals: The Roles of Carbon Side Chains** H.-J. GAO, H.Y. CUN, Y.L. WANG, S.X. DU, L. ZHANG, L.Z. ZHANG, W.A. HOFER, S.J. PENNYCOOK, INSTITUTE OF PHYSICS, CHINESE ACADEMY OF SCIENCES, PR CHINA TEAM, SURFACE SCIENCE RESEARCH CENTRE, UNIVERSITY OF LIVERPOOL, UK COLLABORATION, MATERIALS SCIENCE AND TECHNOLOGY DIVISION, OAK RIDGE NATIONAL LABORATORY, USA COLLABORATION — Organic-molecule based flexible electronics has been of significant interest due to its potential to challenge conventional silicon-based technologies. The crucial properties of these devices rely on the largely invariant physical properties of organic compounds or films when they are mechanically deformed. In this present work, by choosing quinacridone with flexible carbon chains as a model system, we developed a theoretical scheme to evaluate the contributions of various interactions to the molecular self-assembly process and find that such a process should be considered as a collective interaction between molecules and substrates rather than from the viewpoint of an isolated molecule. Importantly, the data provide insight into the origin and an estimate of the magnitude of the Young's modulus of the molecular film, which suggests that the elastic properties of molecular films can be tuned through control of side chain length.

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