Connecting theory with experiment: Raman spectroscopy of organic crystal surfaces

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The surface of a crystal is its interface to the environment and controls important physical properties including the growth morphology, chemical reactivity and dissolution. Understanding the surface chemistry of molecular materials poses a unique challenge, because even simple organic molecules have multiple functional groups that can interact with growth solvents in different ways. Theoretical modelling can provide valuable atomic-level insight into the structure of organic crystal surfaces, but verifying predictions using traditional surface-science techniques is challenging. We have explored the use of Raman spectroscopy to study the major <100> face of aspirin crystals. Guided by theoretical predictions, we show that polarised Raman can be used to selectively enhance spectroscopic signals from surface vibrations, providing a powerful means to identify the functional groups exposed at crystal faces. We demonstrate the application of this technique to understanding the effect of different crystal-growth conditions on the termination of the aspirin <100> surface.