Surface Modification and Functionalizing for Asymmetric Interfaces

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The extremely different bioactivity of the two enantiomers of a chiral species in biological systems has created an enormous demand for enantiopure chemicals in pharmaceutical manufacturing. This has also raised fundamental questions about the origin of biological homochirality in living organisms. It is therefore important to understand chiral environments which can differentiate two enantiomers of a chiral molecule. Solid surfaces can potentially be used for creating chiral environments that are applicable to chiral processing. There are a variety of routes for creating chiral solid surfaces. Surfaces of materials whose bulk crystal structure is enantiomorphic can be used as one type of chiral solid surfaces. Chirality can also be imparted onto surfaces by irreversibly adsorbing chiral organic species on otherwise achiral surfaces. Alternatively, metal surfaces that are intrinsically chiral due to the presence of kinked surface steps provide another route for creating chiral solid surfaces. These surfaces can be created by cutting a single crystal along certain high Miller index directions. We will discuss the enantioselective process to efficiently separate chiral molecules on these types of asymmetric Interfaces using density functional theory calculations.