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# Adsorption of organic molecules on mineral surfaces studied by first-principle calculations: a review

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## Abstract

First-principle calculations, especially by the density functional theory (DFT) methods, are becoming a power technique to study molecular structure and properties of organic/inorganic interfaces. This review introduces some recent examples on the study of adsorption models of organic molecules or oligomers on mineral surfaces and interfacial properties obtained from first-principles calculations. The aim of this contribution is to inspire scientists to benefit from first-principle calculations and to apply the similar strategies when studying and tailoring interfacial properties at the atomistic scale, especially for those interested in the design and development of new molecules and new products.

**Keywords:** First-principle calculations; Density functional theory; Interfacial properties; Adsorption; Mineral surface

**Contents**