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The theory of the chemical interaction of molecules with surfaces has advanced handsomely in the last few years. This is due in part to the application of the entire arsenal of bulk solid-state theory and molecular quantum chemistry methods.

[Theory of chemisorption and reactions on metal surfaces ...](#)

A review of theoretical methods used to describe chemisorption and adsorbate reactions on metal surfaces is contained in this report. A comprehensive perspective on state-of-the-art electronic structure methods suitable for these problems and a review of applications that illustrate current capabilities of theory are presented.

[Theories of Adhesion - adhesion models](#)

Chemisorption theory is an extension of the adsorption theory of adhesion, in which the adhesive has properly wet the substrate, the adhesion phenomenon arises when generating intermolecular or Van der Waals forces and chemical bonds between the adhesive and substrate.

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The theory of the chemical interaction of molecules with surfaces has advanced handsomely in the last few years. This is due in part to the application of the entire arsenal of bulk solid-state theory and molecular quantum chemistry methods. This considerable activity was stimulated by an [Induced covalent bond theory of chemisorption - ScienceDirect](#)

The theory of the induced covalent bond mechanism for free radical chemisorption on a metal surface is developed as a hybrid between the molecular orbital for the substrate and the Heitler-London scheme for the adsorbate.

[A oneelectron perturbation theory of chemisorption](#)

A one-electron perturbation theory of chemisorption Mikhail V. Basilevsky Karpov Institute of Physical Chemistry, Ul. Obukha 10, 103064 Moscow K-64.

[Theory of Chemisorption ; J. R. Smith ; 9783642814334](#)

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[Chemisorption - Wikipedia](#)

Chemisorption is a kind of adsorption which involves a chemical reaction between the surface and the adsorbate. New chemical bonds are generated at the adsorbant surface. Examples include macroscopic phenomena that can be very obvious, like

[Adsorption Isotherm \(Theory\) : Physical Chemistry](#)

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Theory: Adhesion of atoms, ions, bimolecules or molecules of gas, liquid or dissolved solids to a surface is called adsorption. This process creates a film of the adsorbate the molecules or atoms being accumulated, on the surface of the adsorbent.

Physisorption - Wikipedia

Physisorption, also called physical adsorption, is a process in which the electronic structure of the atom or molecule is barely perturbed upon adsorption.

Quantum Theory of Dissociative Chemisorption on Metal Surfaces

Quantum Theory of Dissociative Chemisorption on Metal Surfaces GEERT-JAN KROES,* AXEL GROSS, EVERT-JAN BAERENDS, MATTHIAS SCHEFFLER, AND

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The electronic structure of a semiinfinite crystal with a partial coverage by adatoms is studied within the tight-binding formalism. The effect of the surface is described via the surface Green function method, and the effect of disorder is treated within the coherent potential approximation. The

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