EPFL
École polytechnique fédérale de Lausanne

Institute of Materials - Institute of Bioengineering
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SuNMiL
Supramolecular NanoMaterials and Interfaces Laboratory

Electronic Properties of Surfaces
Lesson 13

MSE 304

Francesco Stellacci

桑缪 썬밀 सानमिल ΣουNMιΛ سنمل СаНМПЛ

Reading for this Class

Chapter 5 and 6 of “Introduction to Surface Chemistry and Catalysis” by G. Samorjai

Key Topics from the Course

Concept of Surface

Key Topics from the Course

Diffuse Interfaces

Key Topics from the Course

Adsorbates on Surfaces

Key Topics from the Course

Charged Interfaces

Content of this Class

Content of this Class

Solid State Electronic Description

Surface Electronic Description

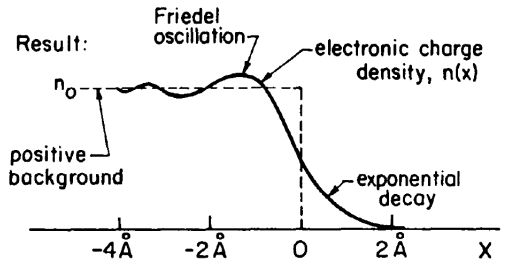


Figure 5.1. Schematic representation of the electronic charge density distribution at a metal surface.

Charge Density at Interfaces

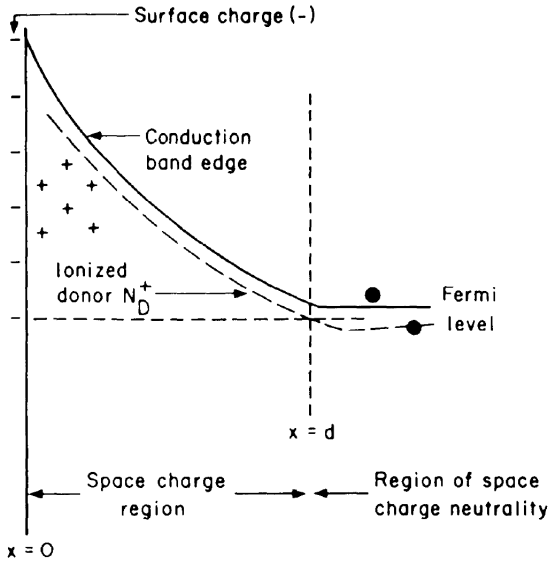


Figure 5.2. Scheme of space-charge buildup at an *n*-type semiconductor surface upon adsorption of electron acceptor molecules.

$$\frac{d^2V}{dx^2} = -\frac{\rho_e(x)}{\epsilon\epsilon_0}$$

$$V(x) = -\frac{e}{2\epsilon\epsilon_0} N_D^+ (x - d)^2$$

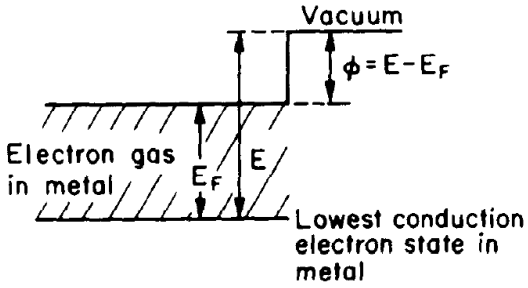
$$V_s = \frac{e}{2\epsilon\epsilon_0} N_D^+ d^2$$

$$en_e^{\text{bulk}} d \approx eN_D^+ d$$

$$d = \left[\frac{2\epsilon\epsilon_0 V_s}{en_e^{\text{bulk}}}\right]^{1/2}$$

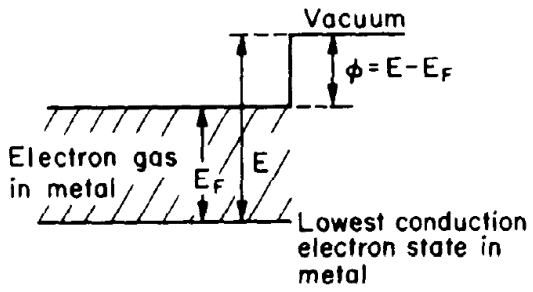
The Work Function

The Work Function in a Realistic Sample



$$e\phi = eV_{\text{exchange}} + eV_{\text{dipole}} - E_F$$

The Work Function in a Realistic Sample



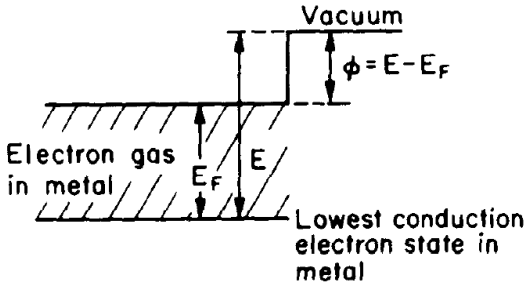
$$e\phi = eV_{\text{exchange}} + eV_{\text{dipole}} - E_F$$

Dependence on Facets

Dependence on Size

Dependence on Roughnes

The Work Function in a Realistic Sample



$$e\phi = eV_{\text{exchange}} + eV_{\text{dipole}} - E_F$$

Adsorption at Surfaces: Charge Transfer

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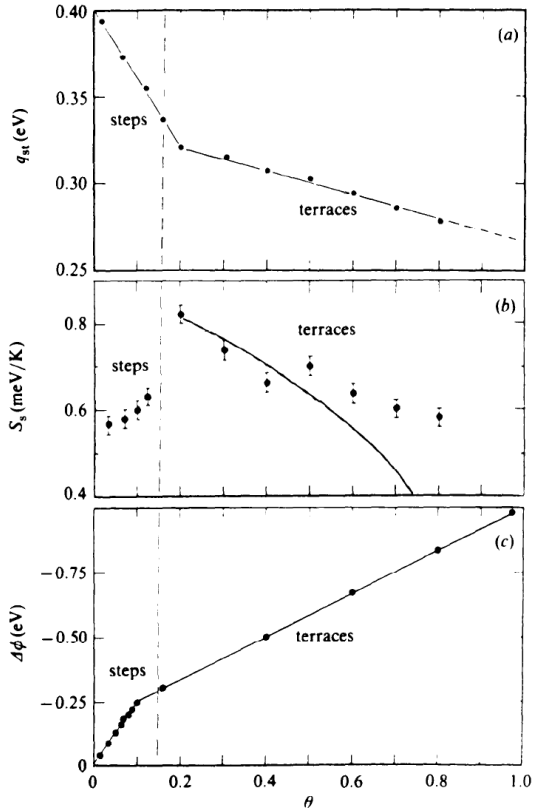


Figure 5.6. The enthalpy change **(a)**, the entropy **(b)**, and the work function change **(c)** for xenon adsorption as a function of xenon coverage on the Pd(810) stepped crystal surface [53].

Work Function and Adsorption

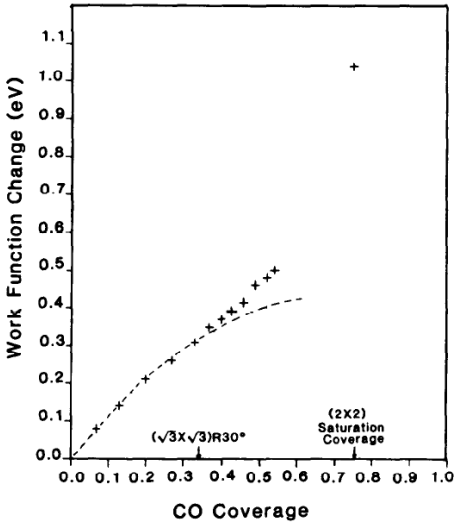


Figure 5.7. The change of work function of Rh(111) upon CO adsorption as a function of coverage [54].

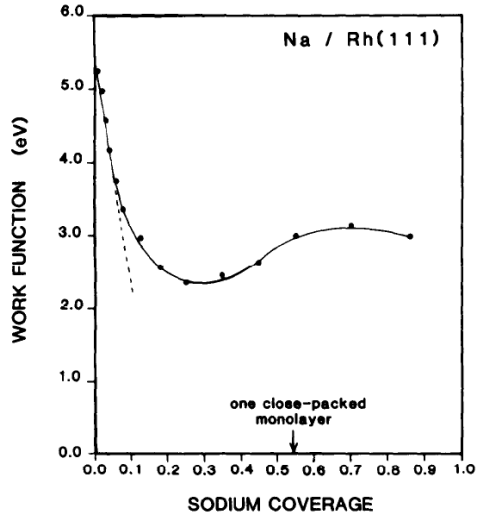
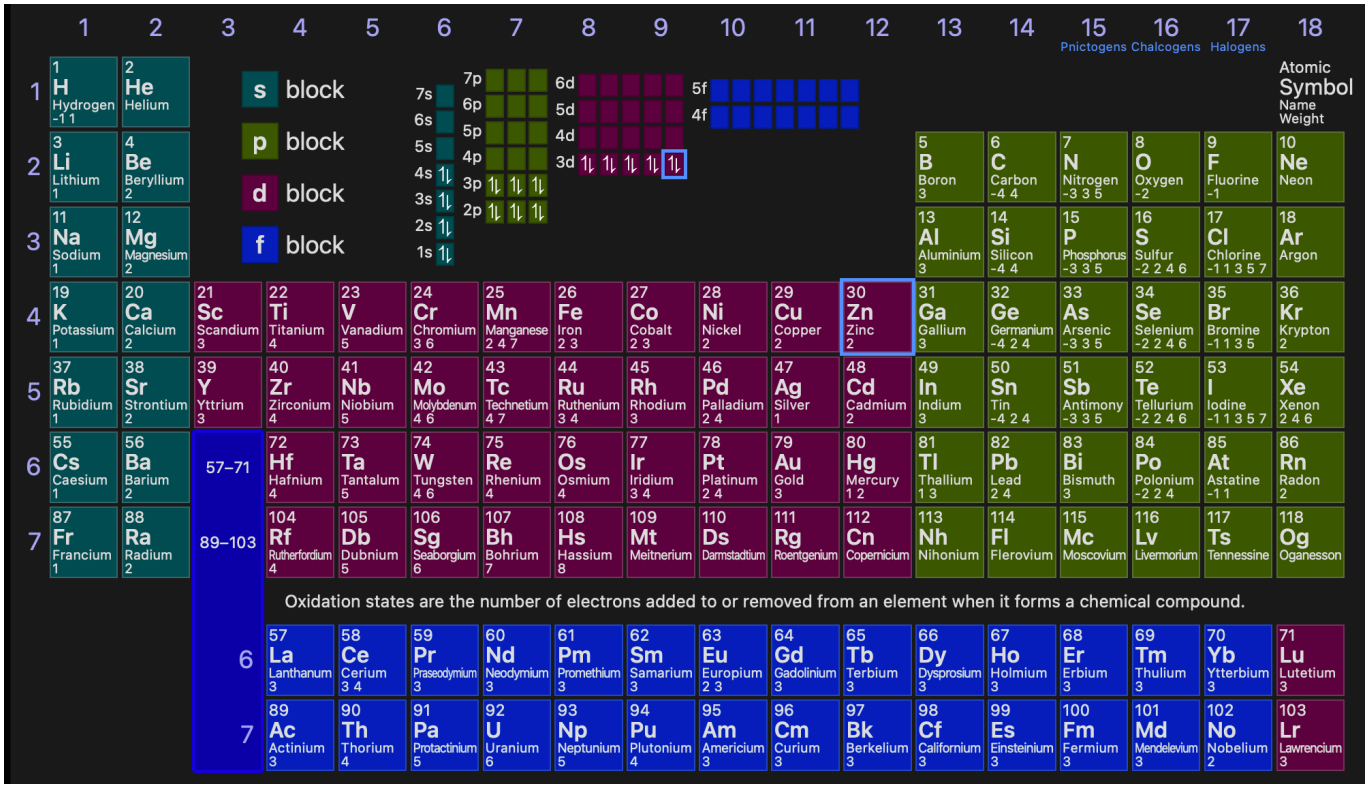
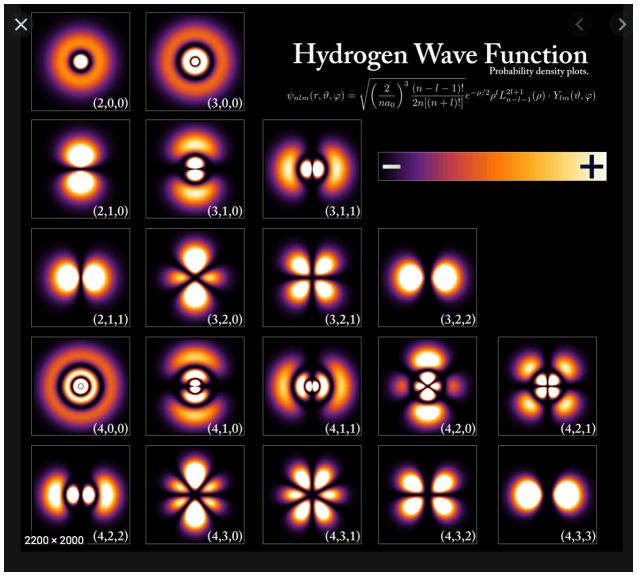


Figure 5.8. The change of work function of Rh(111) upon adsorption of sodium as a function of Na coverage [54].

Adsorption vs Absorption

The Periodic Table





https://ptable.com/?lang=en#Electrons

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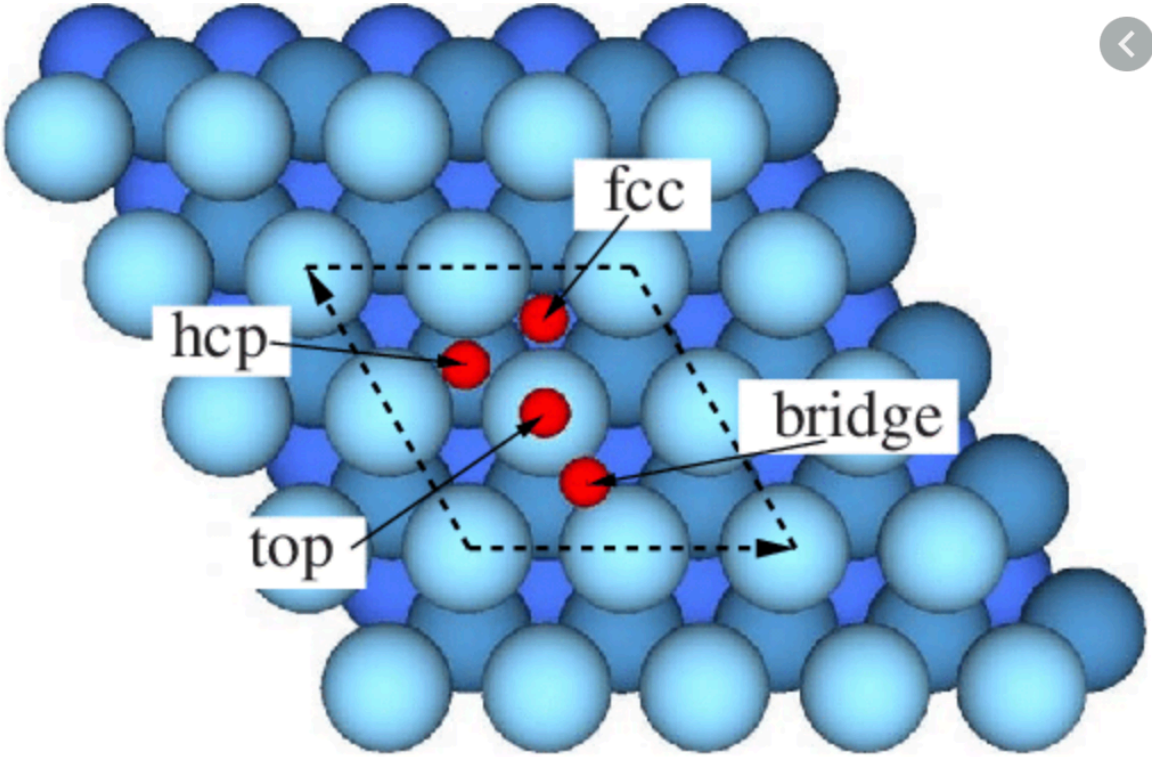
The Molecular Orbital Theory

Bands in Solids

Absorption on Solids

Absorption Geometry



The Chemical Bond

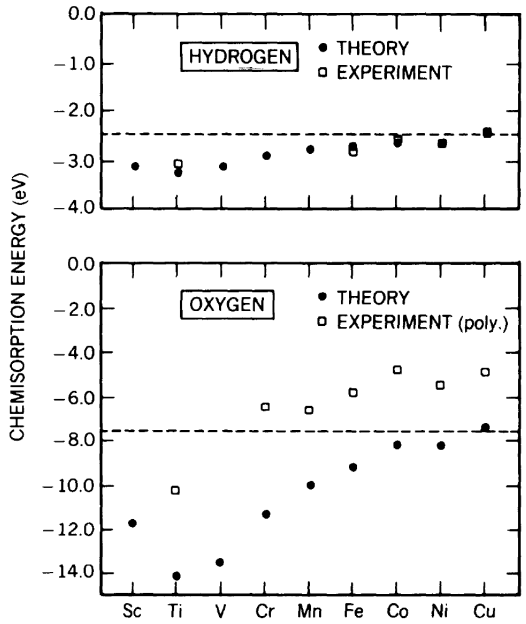
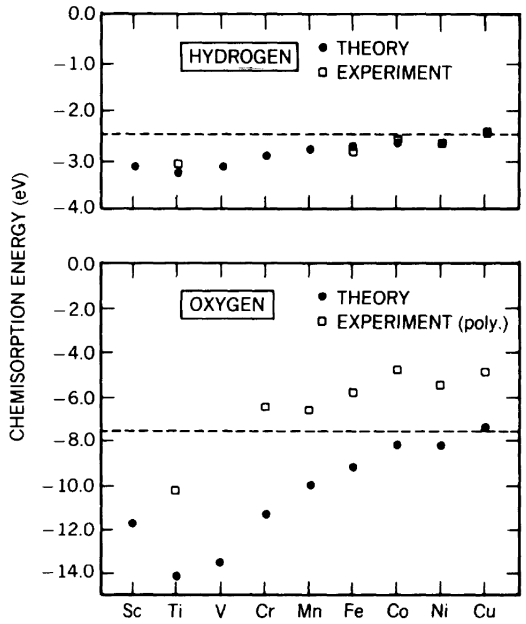


Figure 6.1. Chemisorption energies of hydrogen and oxygen on transition metals across the periodic table that were calculated using the effective-medium theory and also measured on polycrystalline surfaces [23].

The Chemical Bond



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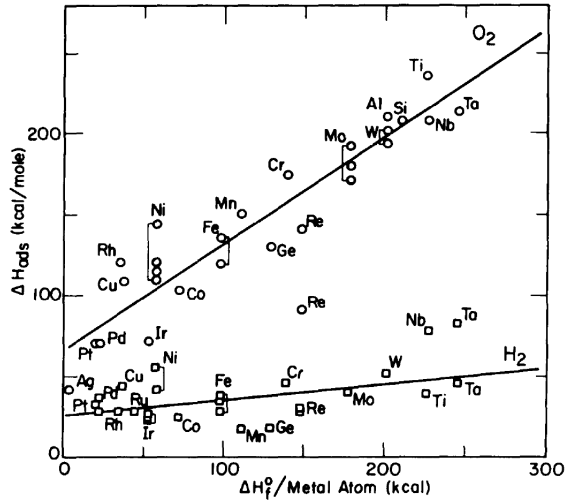


Figure 6.2. Heats of adsorption of O_2 and H_2 on various transition metals as a function of the heats of formation of the corresponding oxides and hydrides (per metal atom) [2].

The Chemical Bond

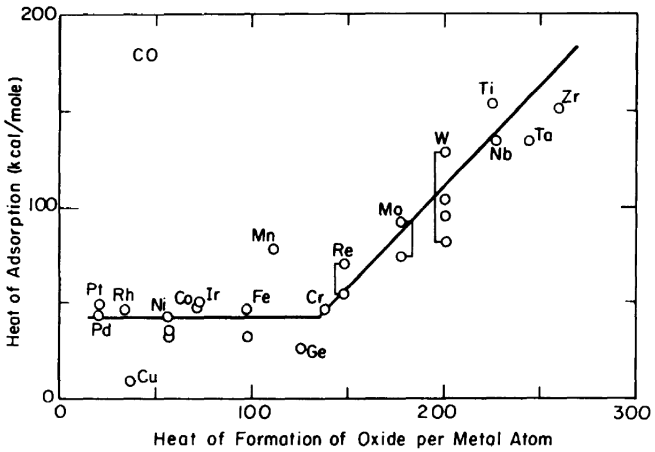
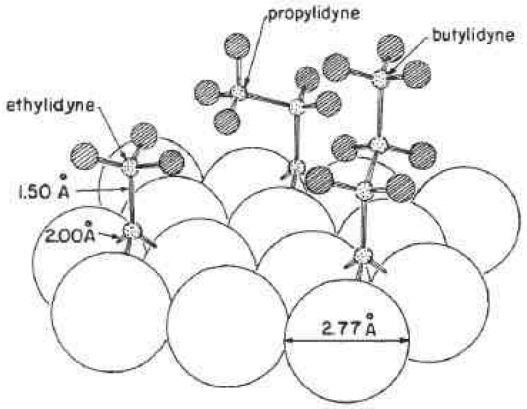


Figure 6.3. Heats of adsorption of CO on various transition metals as a function of the heats of formation of the corresponding oxides (per metal atom) [2].

The Chemical Bond



Pt (111) + ethylidyne, propylidyne and butylidyne

The Chemical Bond- Absorption on Surfaces

Gas Separation

Materials with high Surface Area to Volume Ratio

Conclusions