

Electronic Properties of Surfaces

Lesson 13

MSE 304

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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

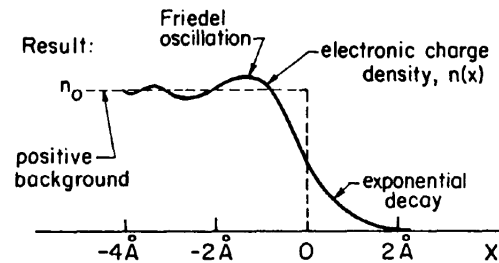


Figure 5.1. Schematic representation of the electronic charge density distribution at a metal surface.

Charge Density at Interfaces

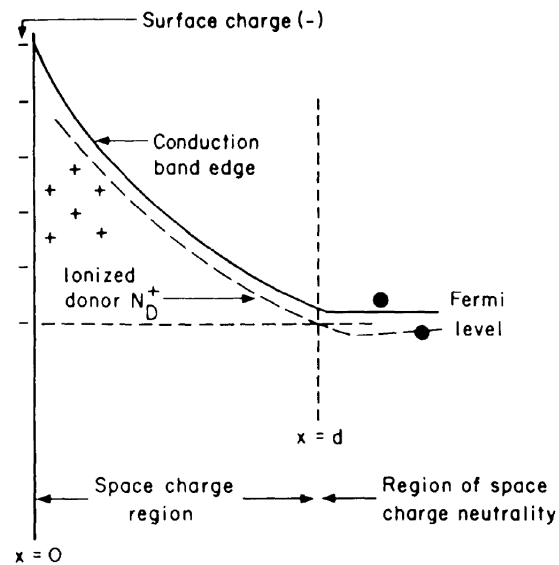


Figure 5.2. Scheme of space-charge buildup at an *n*-type semiconductor surface upon adsorption of electron acceptor molecules.

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

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

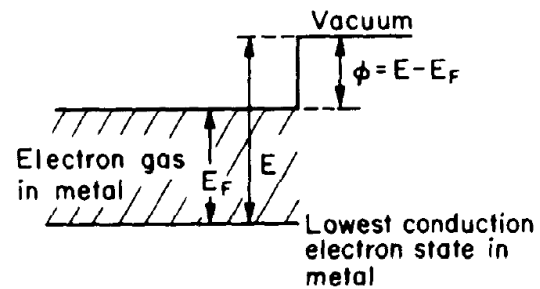
$$V_s = \frac{e}{2\epsilon\epsilon_0} N_D^+ d^2$$

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

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

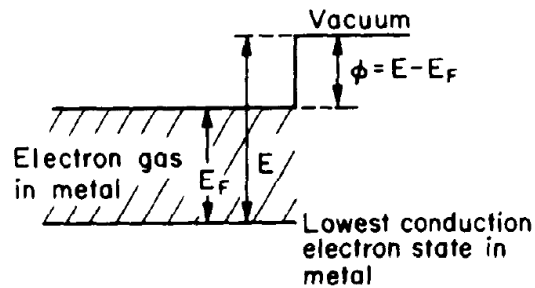
The Work Function

The Work Function in a Realistic Sample



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

The Work Function in a Realistic Sample



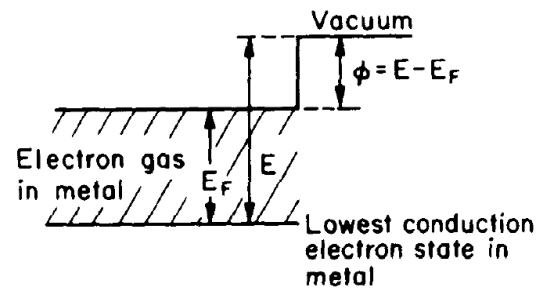
$$e\phi = eV_{\text{exchange}} + eV_{\text{dipole}} - E_F$$

Dependence on Facets

Dependence on Size

Dependence on Roughness

The Work Function in a Realistic Sample



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

Adsorption at Surfaces: Charge Transfer

Adsorption at Surfaces: Charge Transfer

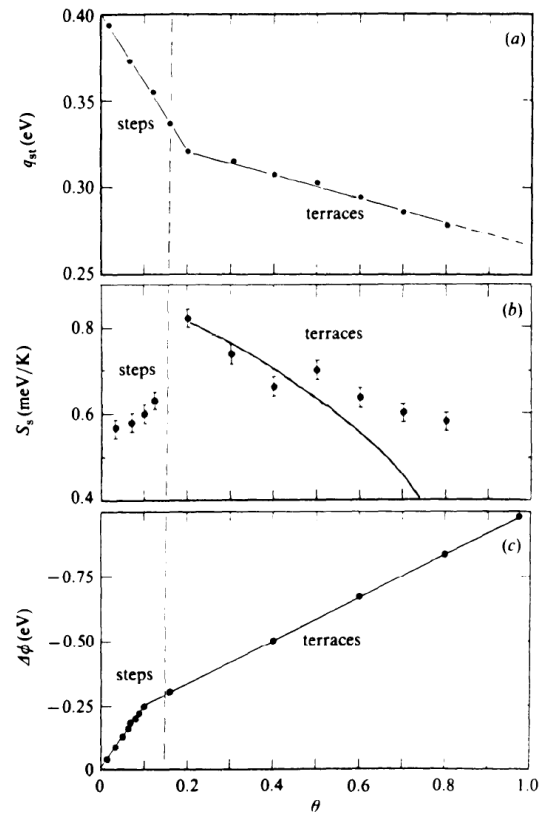


Figure 5.6. The enthalpy change (a), the entropy (b), and the work function change (c) for xenon adsorption as a function of xenon coverage on the Pd(810) stepped crystal surface [53].

Work Function and Adsorption

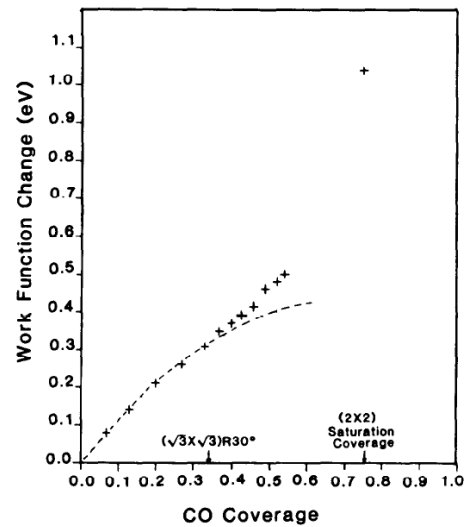


Figure 5.7. The change of work function of Rh(111) upon CO adsorption as a function of coverage [54].

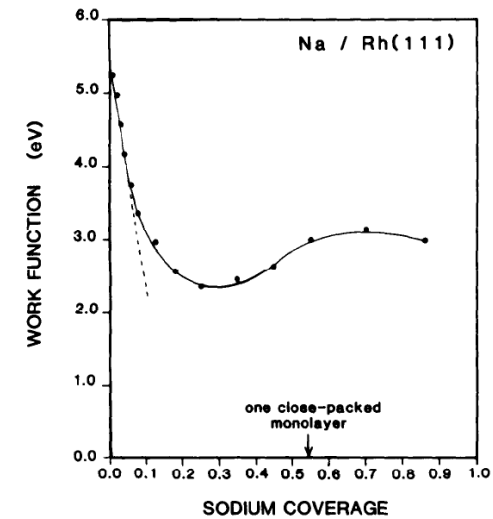


Figure 5.8. The change of work function of Rh(111) upon adsorption of sodium as a function of Na coverage [54].

Adsorption vs Absorption

The Periodic Table

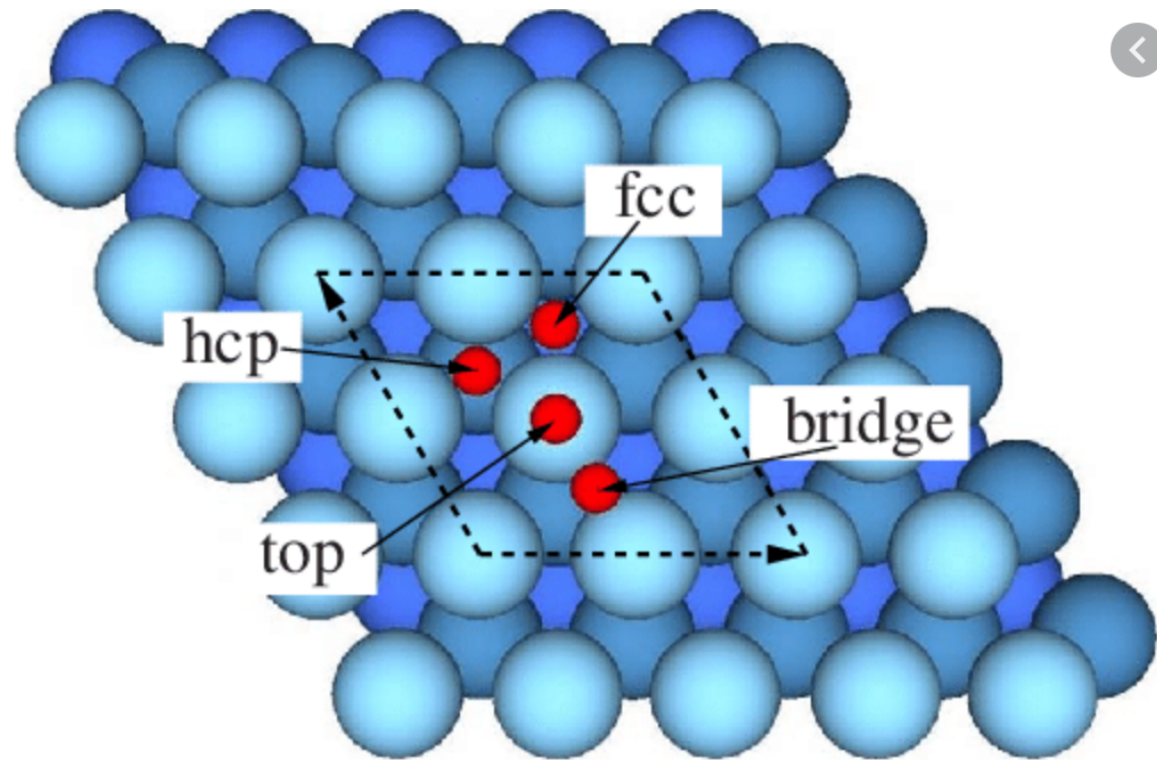
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	
			Periodic Table of Elements																Atomic Symbol
			Periodic Table of Elements																Name Weight
1	1 H Hydrogen -1.1	2 He Helium																	
2	3 Li Lithium 1	4 Be Beryllium 2																	
3	11 Na Sodium 1	12 Mg Magnesium 2																	
4	19 K Potassium 1	20 Ca Calcium 2	21 Sc Scandium 3	22 Ti Titanium 4	23 V Vanadium 5	24 Cr Chromium 3 6	25 Mn Manganese 2 4 7	26 Fe Iron 2 3	27 Co Cobalt 2 3	28 Ni Nickel 2	29 Cu Copper 2	30 Zn Zinc 2	31 Ga Gallium 3	32 Ge Germanium -4 2 4	33 As Arsenic -3 3 5	34 Se Selenium -2 2 4 6	35 Br Bromine -1 1 3 5	36 Kr Krypton 2	
5	37 Rb Rubidium 1	38 Sr Strontium 2	39 Y Yttrium 3	40 Zr Zirconium 4	41 Nb Niobium 5	42 Mo Molybdenum 4 6	43 Tc Technetium 4 7	44 Ru Ruthenium 3 4	45 Rh Rhodium 3 4	46 Pd Palladium 2 4	47 Ag Silver 1	48 Cd Cadmium 2	49 In Indium 3	50 Sn Tin -4 2 4	51 Sb Antimony -3 3 5	52 Te Tellurium -2 2 4 6	53 I Iodine -1 1 3 5 7	54 Xe Xenon 2 4 6	
6	55 Cs Caesium 1	56 Ba Barium 2	57-71		72 Hf Hafnium 4	73 Ta Tantalum 5	74 W Tungsten 4 6	75 Re Rhenium 4	76 Os Osmium 4	77 Ir Iridium 3 4	78 Pt Platinum 2 4	79 Au Gold 3	80 Hg Mercury 1 2	81 Tl Thallium 1 3	82 Pb Lead 2 4	83 Bi Bismuth 3	84 Po Polonium -2 2 4	85 At Astatine -1 1	86 Rn Radon 2
7	87 Fr Francium 1	88 Ra Radium 2	89-103		104 Rf Rutherfordium 4	105 Db Dubnium 5	106 Sg Seaborgium 6	107 Bh Bohrium 7	108 Hs Hassium 8	109 Mt Meitnerium 7	110 Ds Darmstadtium 8	111 Rg Roentgenium 7	112 Cn Copernicium 8	113 Nh Nihonium 7	114 Fl Flerovium 8	115 Mc Moscovium 7	116 Lv Livermorium 8	117 Ts Tennessine 7	118 Og Oganesson 8
	Oxidation states are the number of electrons added to or removed from an element when it forms a chemical compound.																		
			6		57 La Lanthanum 3	58 Ce Cerium 3 4	59 Pr Praseodymium 3	60 Nd Neodymium 3	61 Pm Promethium 3	62 Sm Samarium 2 3	63 Eu Europium 2 3	64 Gd Gadolinium 3	65 Tb Terbium 3	66 Dy Dysprosium 3	67 Ho Holmium 3	68 Er Erbium 3	69 Tm Thulium 3	70 Yb Ytterbium 3	71 Lu Lutetium 3
			7		89 Ac Actinium 3	90 Th Thorium 4	91 Pa Protactinium 5	92 U Uranium 6	93 Np Neptunium 4	94 Pu Plutonium 4	95 Am Americium 3	96 Cm Curium 3	97 Bk Berkellium 3	98 Cf Californium 3	99 Es Einsteinium 3	100 Fm Fermium 3	101 Md Mendelevium 3	102 No Nobelium 2	103 Lr Lawrencium 3

The Molecular Orbital Theory

Bands in Solids

Absorption on Solids

Absorption Geometry



The Chemical Bond

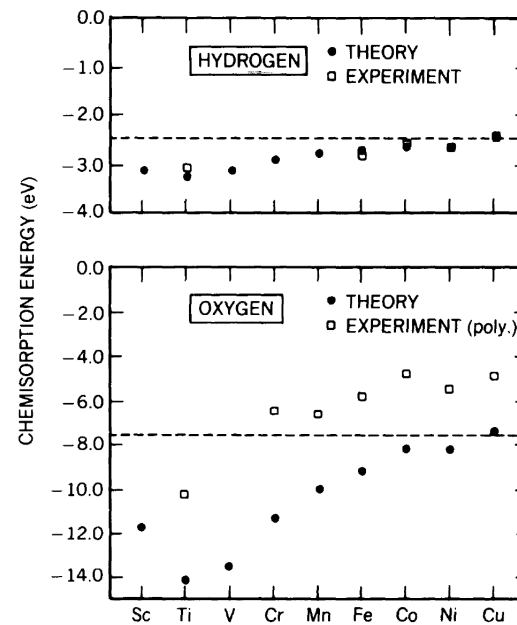


Figure 6.1. Chemisorption energies of hydrogen and oxygen on transition metals across the periodic table that were calculated using the effective-medium theory and also measured on polycrystalline surfaces [23].

The Chemical Bond

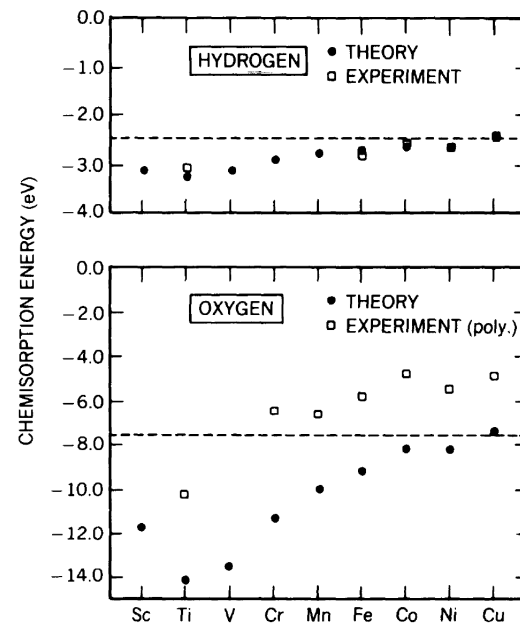


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The Chemical Bond

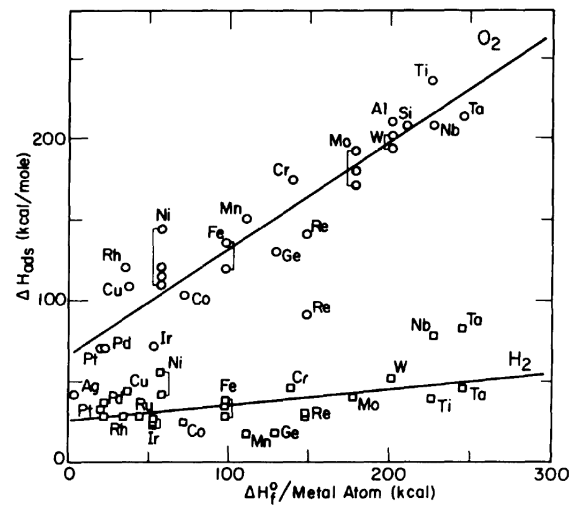


Figure 6.2. Heats of adsorption of O_2 and H_2 on various transition metals as a function of the heats of formation of the corresponding oxides and hydrides (per metal atom) [2].

The Chemical Bond

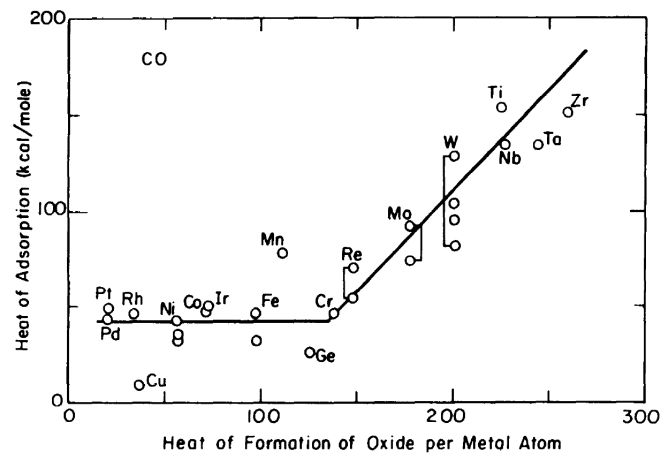
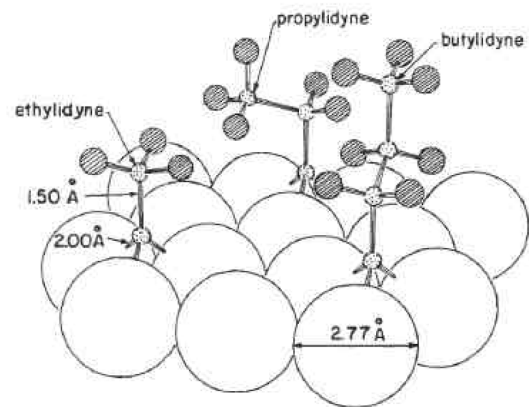


Figure 6.3. Heats of adsorption of CO on various transition metals as a function of the heats of formation of the corresponding oxides (per metal atom) [2].

The Chemical Bond



Pt(III) + ethynylidyne, propynylidyne and butynylidyne

The Chemical Bond- Absorption on Surfaces

Gas Separation

Materials with high Surface Area to Volume Ratio

Conclusions
