

Relevancia de estructuras cristalinas

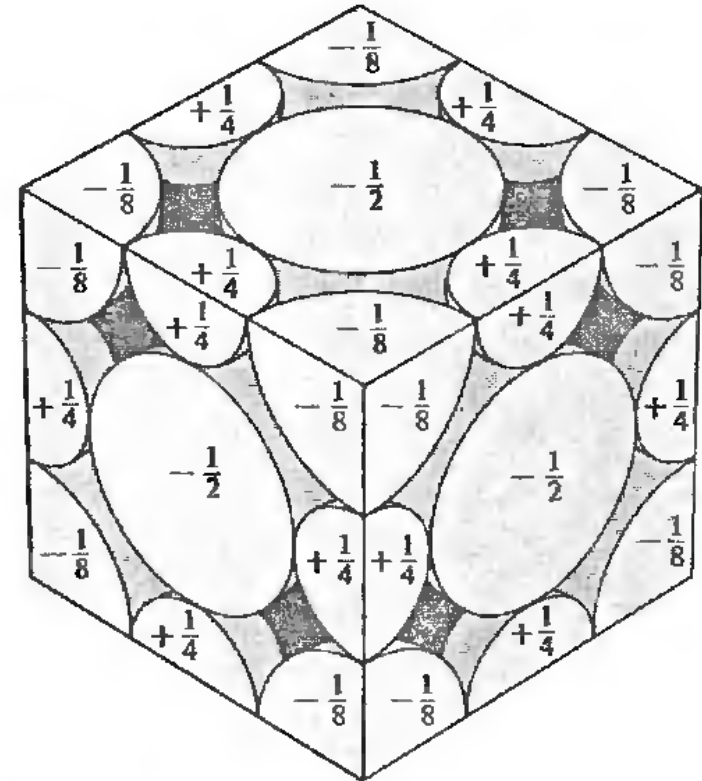
Mecanicas

Opticas

Magneticas

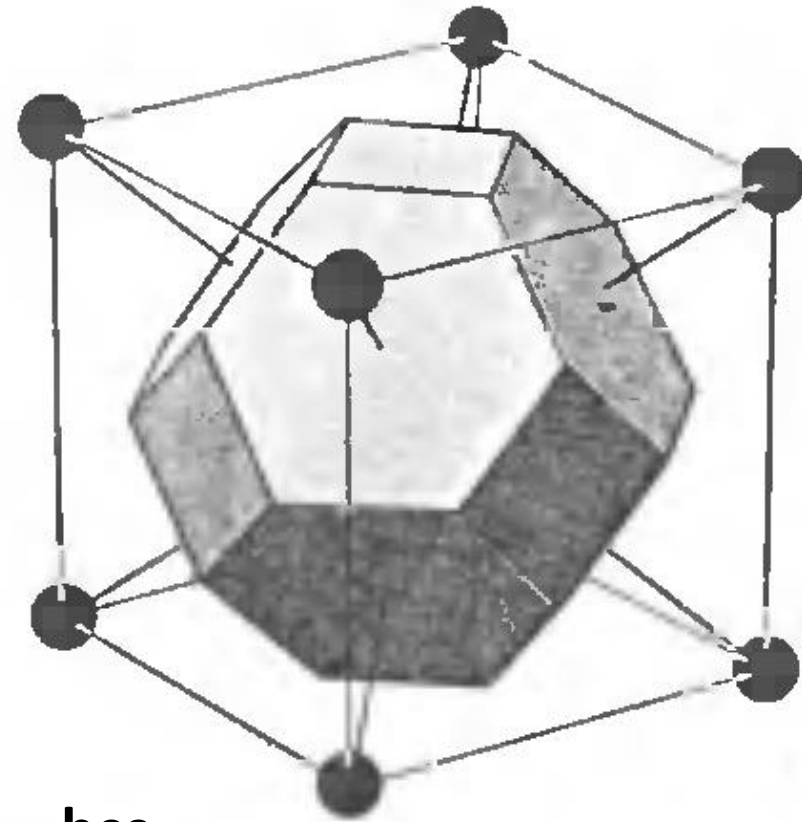
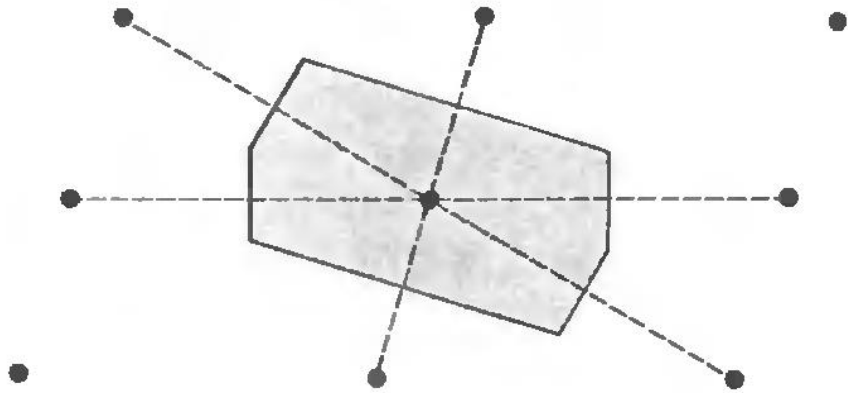
Electricas

Anisotropias



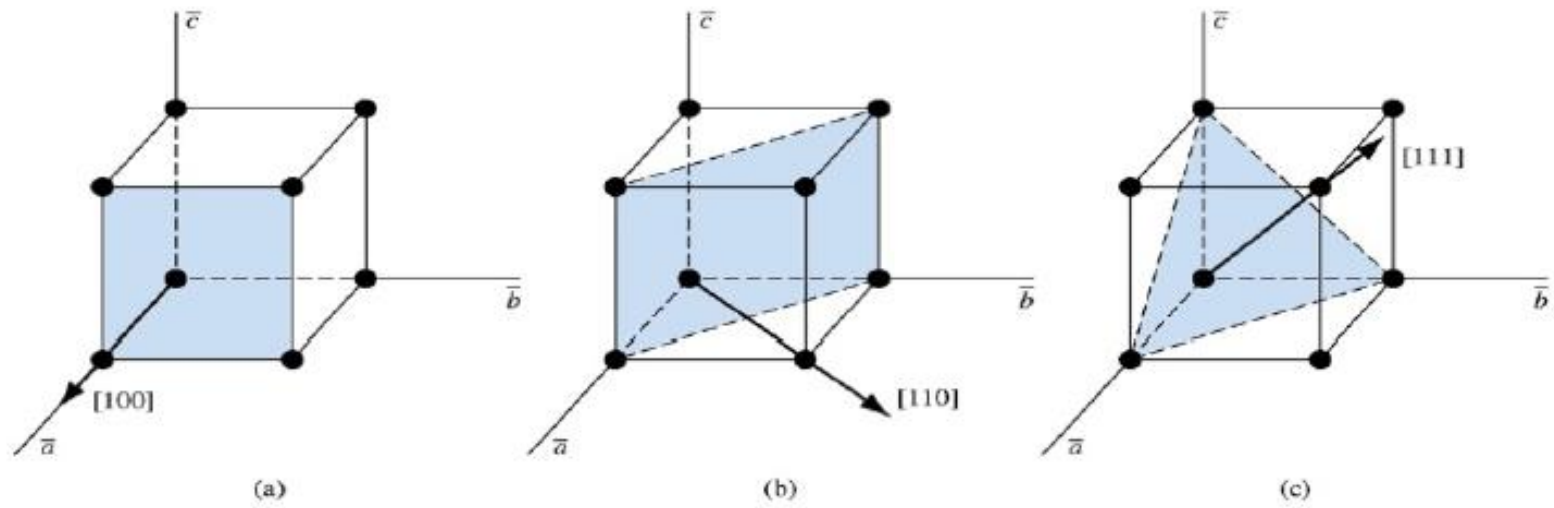
Definiciones

Celda de Wigner Seitz



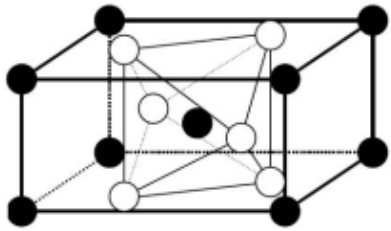
bcc

Ej. de planos mas relevantes de una estructura cubica

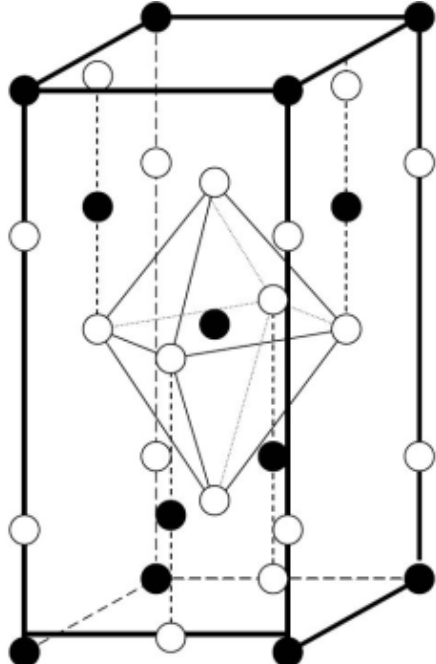


Importancia de la estructura cristalina. Ej. TiO₂

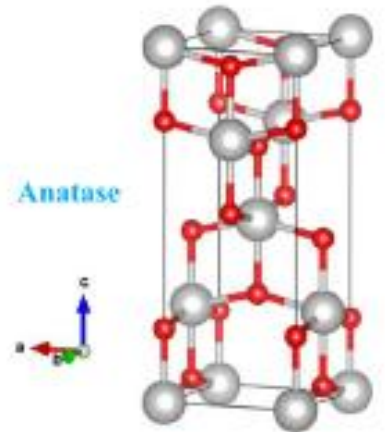
● Titanium
○ Oxygen



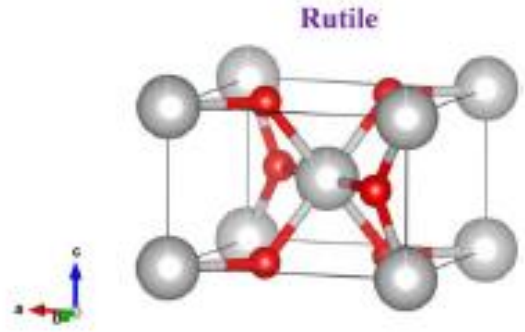
Rutile



Anatase



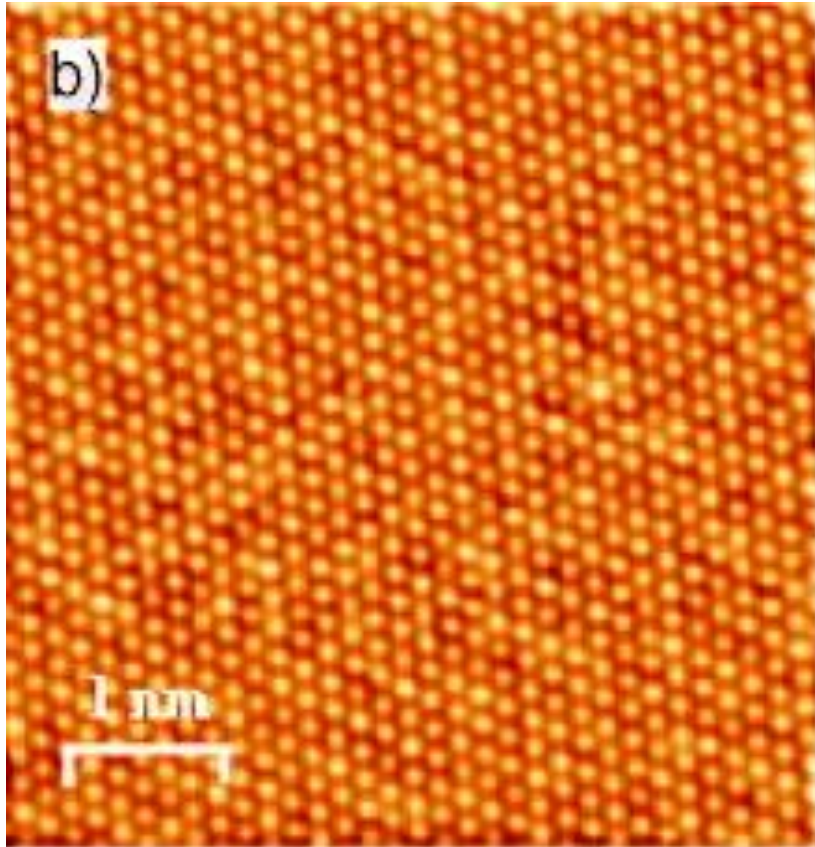
Anatase



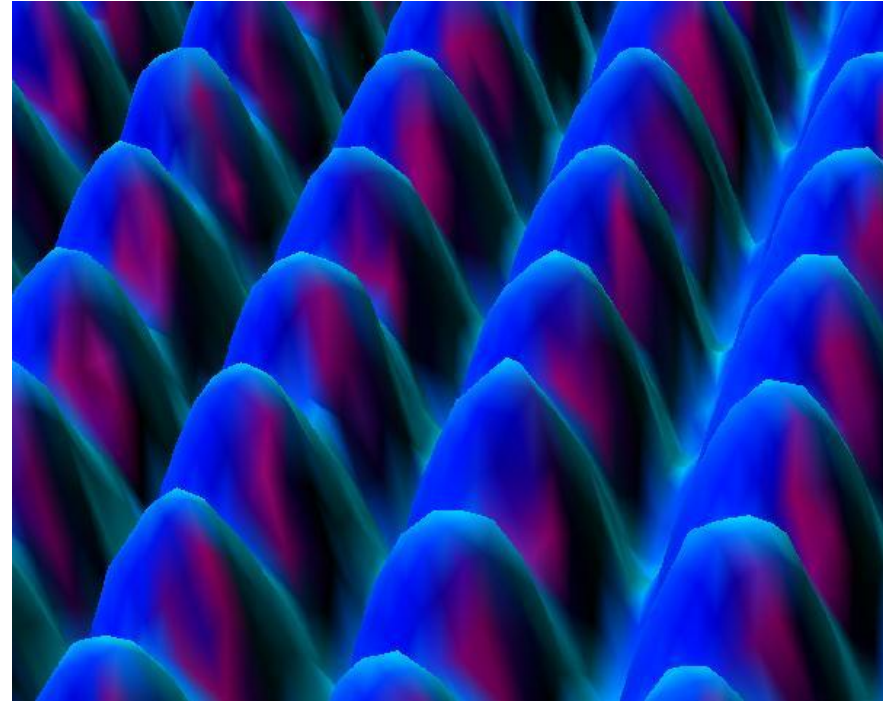
Rutile

ADSORCION

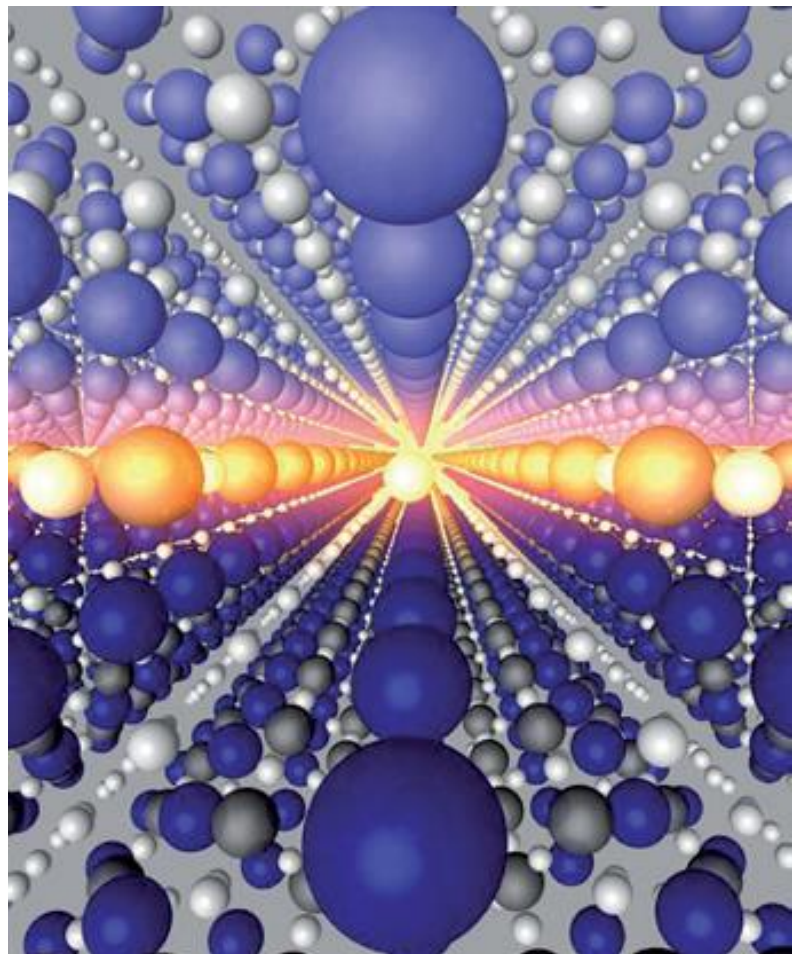
Superficie de Pb



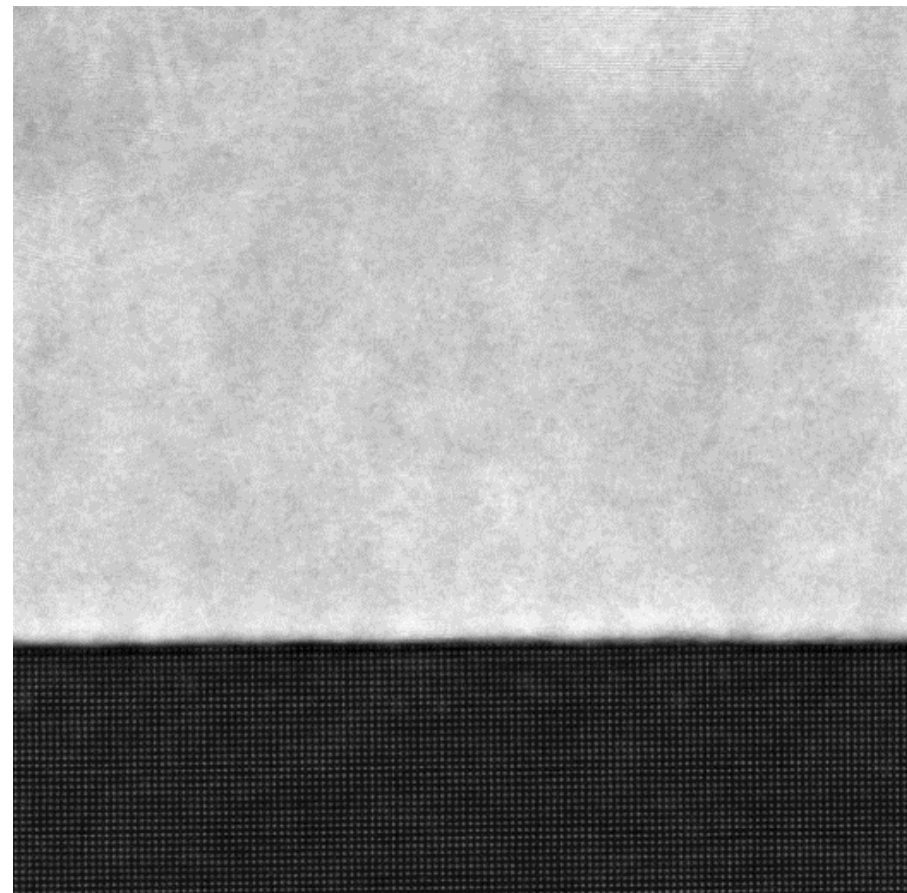
Pt (IBM Almaden USA)



INTERFACES

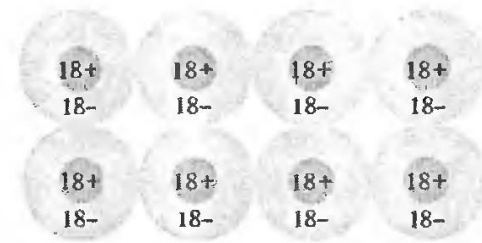


FePt/BaTiO₃ LNMD-INN

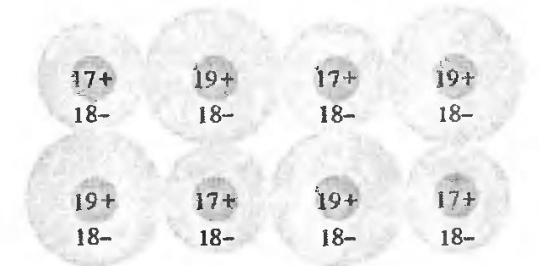


LIGADURAS EN UN SOLIDO

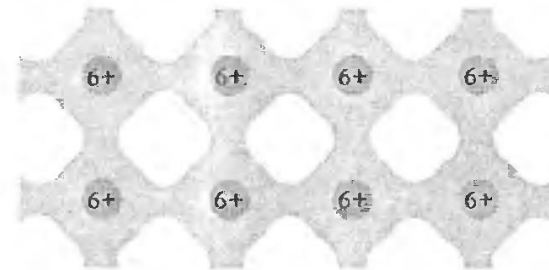
- Dipolo-dipolo => cristales moleculares
- Iónica => cristales ionicos
- Covalente => cristales covalentes (aislantes o semiconductores)
- Metálica => metales



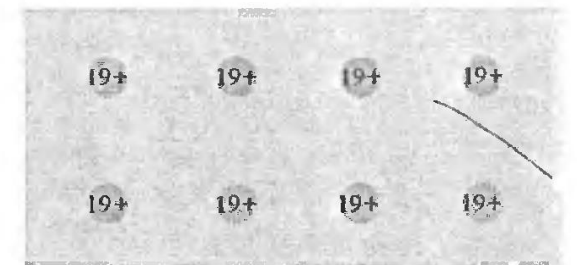
Molecular
(a)



Ionic
(b)

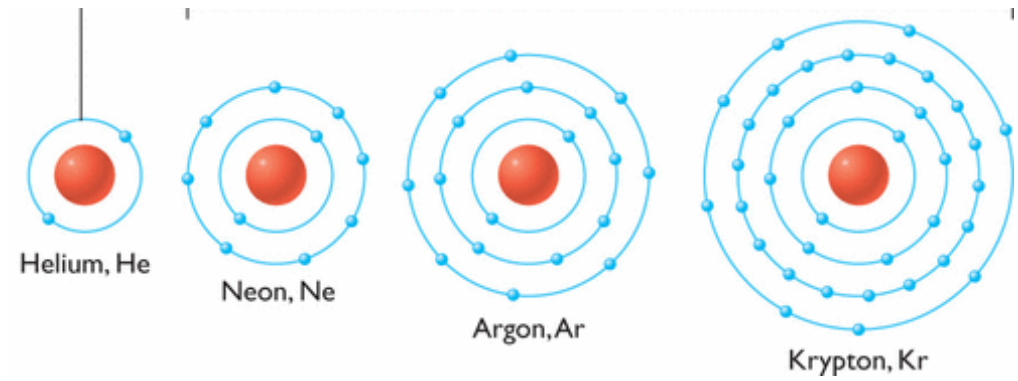


Covalent
(c)



Metallic
(d)

Solidos de gases nobles



A 1atm presión > se pueden condensar en estructuras fcc

Temperatura de fusion

Neon 24.5 K

Argon 84 K

Krypton 116 K

Xenon 161 K

Radon 202 K

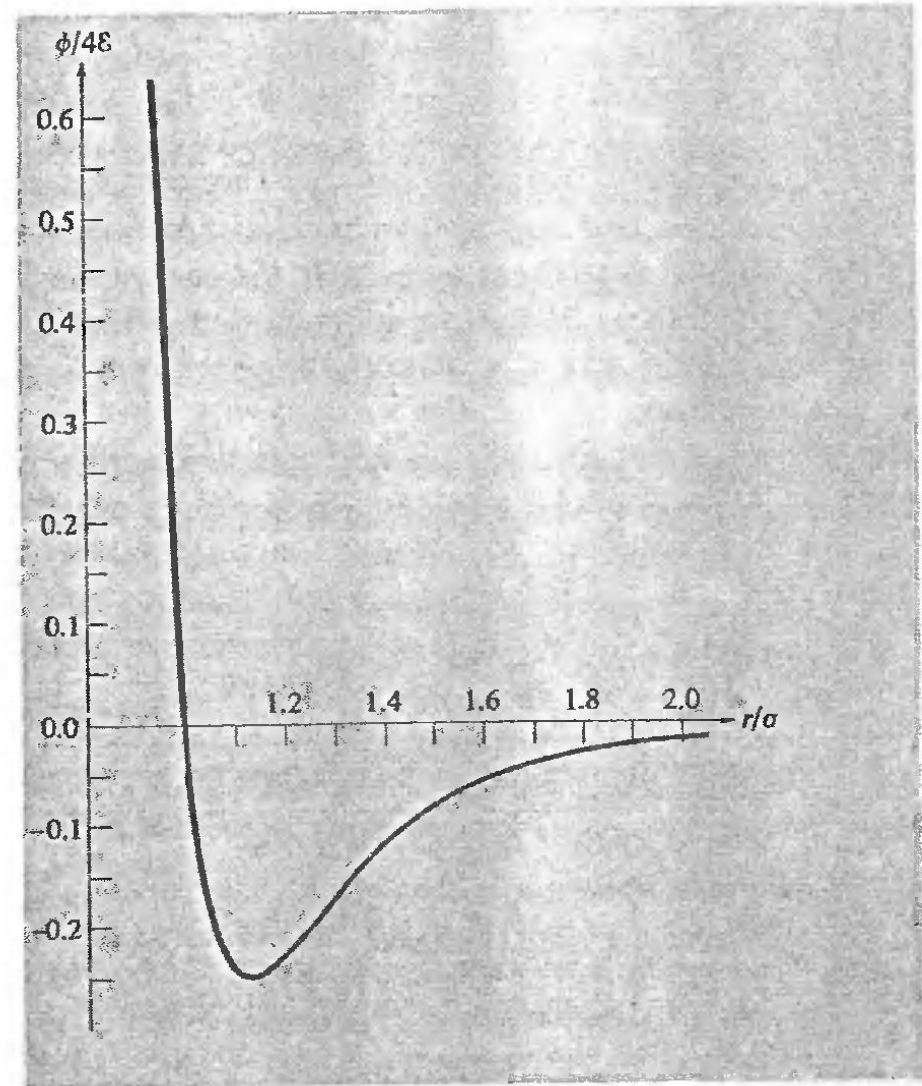
interaccion de Van der Waals

dipole-dipolo

Potencial de Lennard Jones

cristales moleculares

2

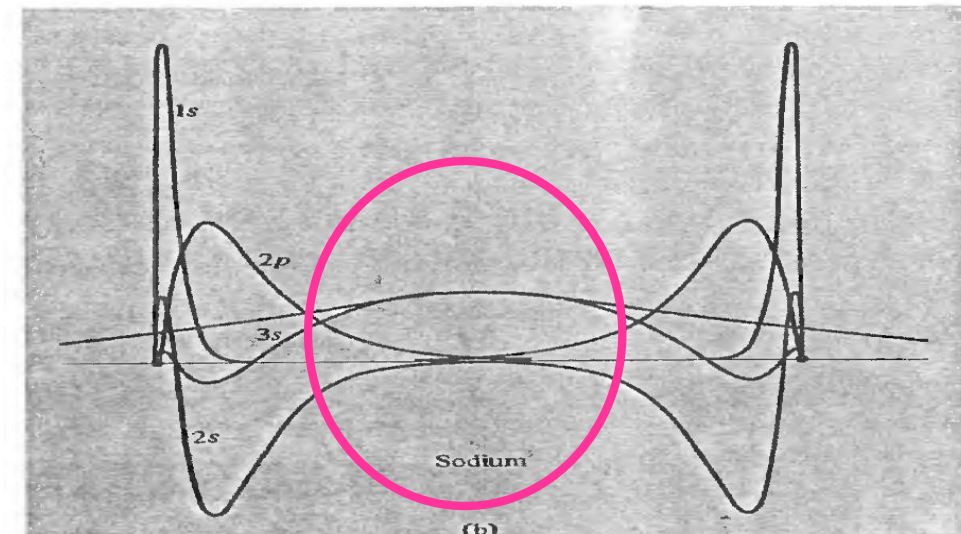
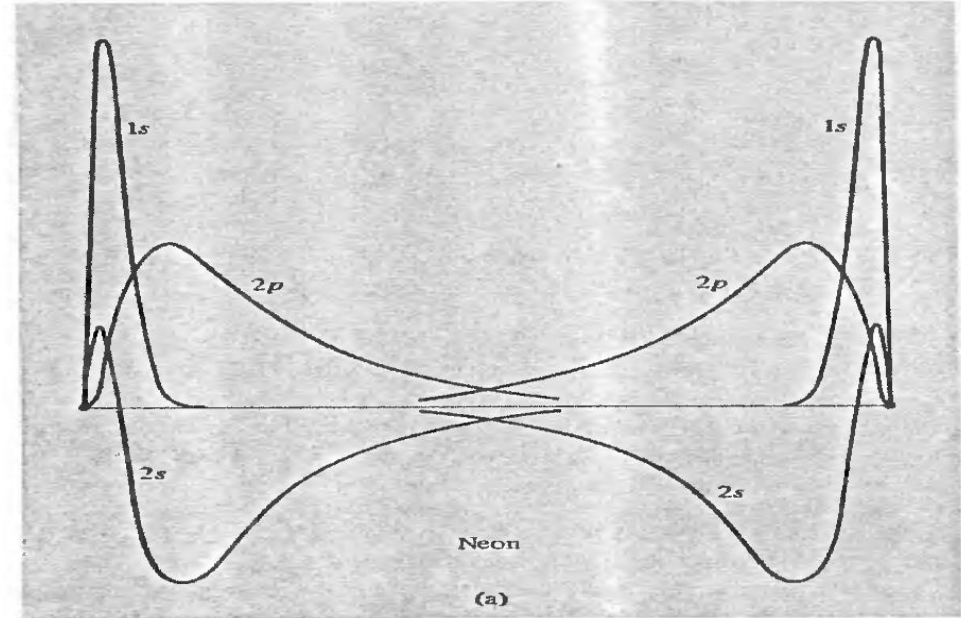


Funcion de onda atómica radial calculada para Ne y Na

Ne $1s^2 2s^2 2p^6$ (3.1A)

y Na $1s^2 2s^2 2p^6 3s^1$ (3.7A)

Centradas en sitios de primeros vecinos



Uniones iónicas

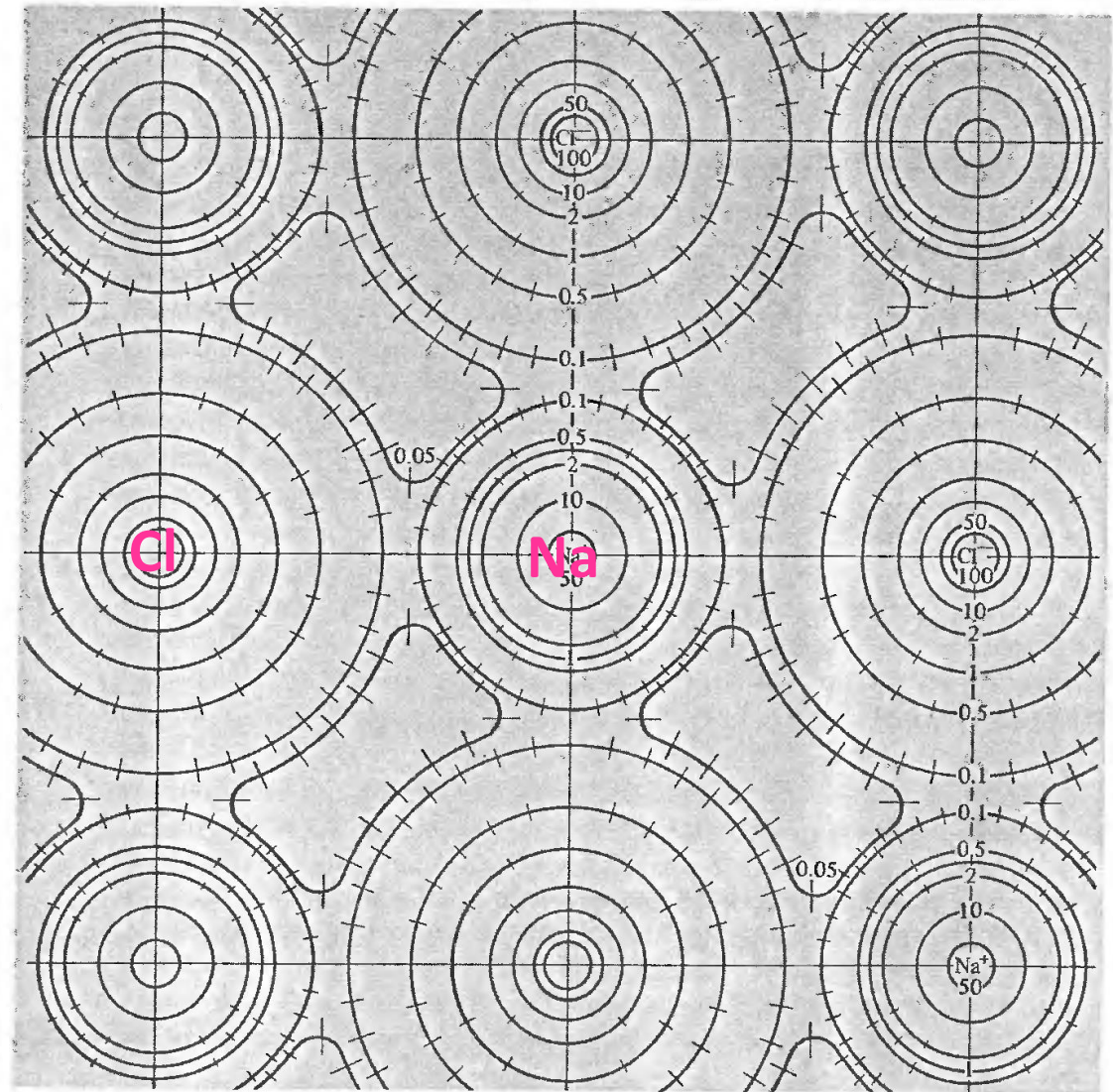
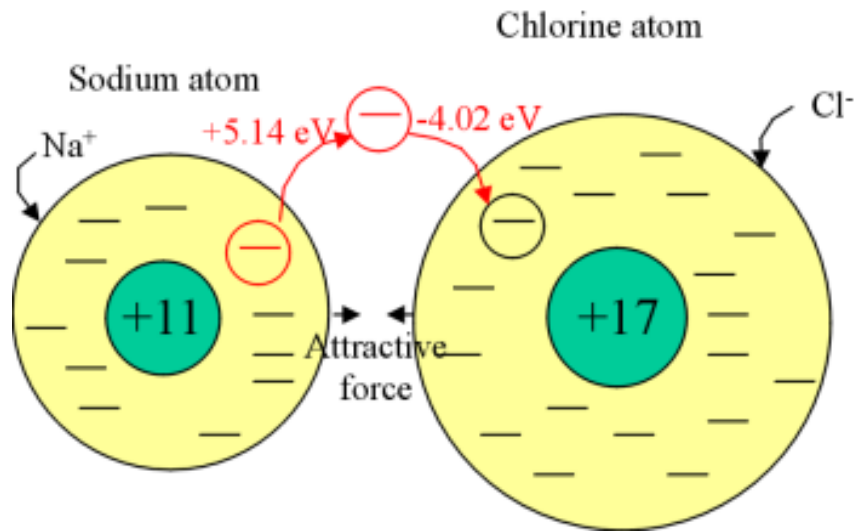
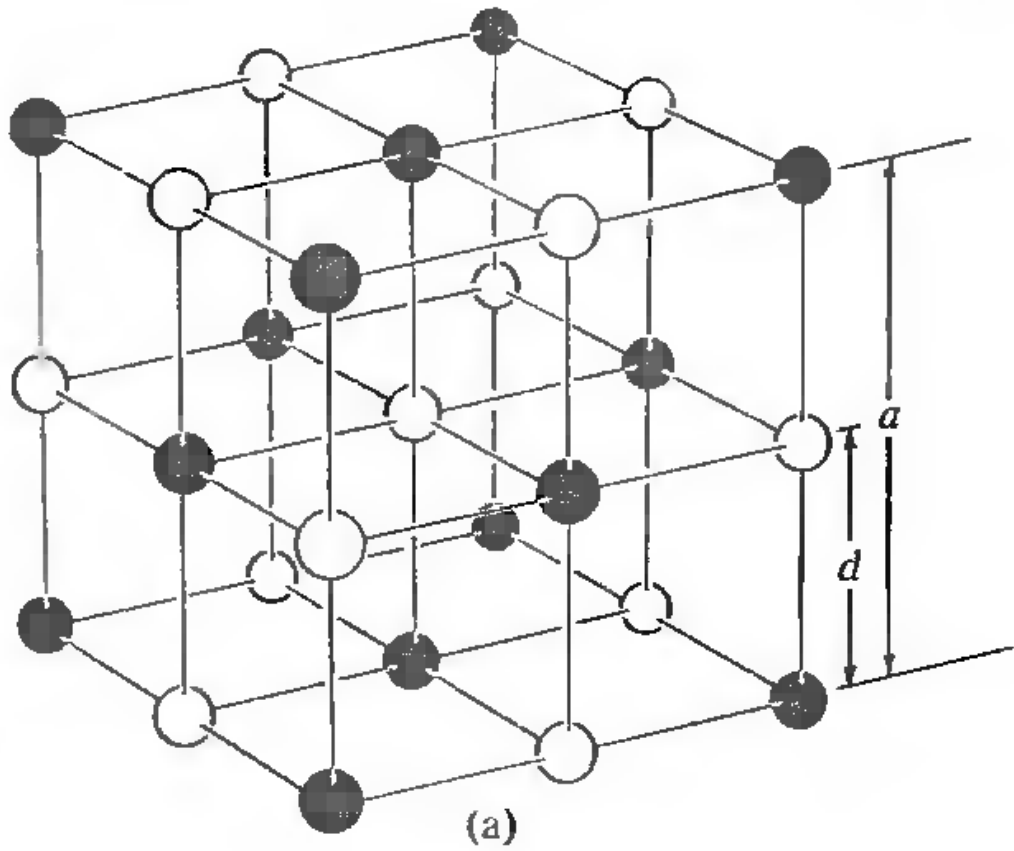
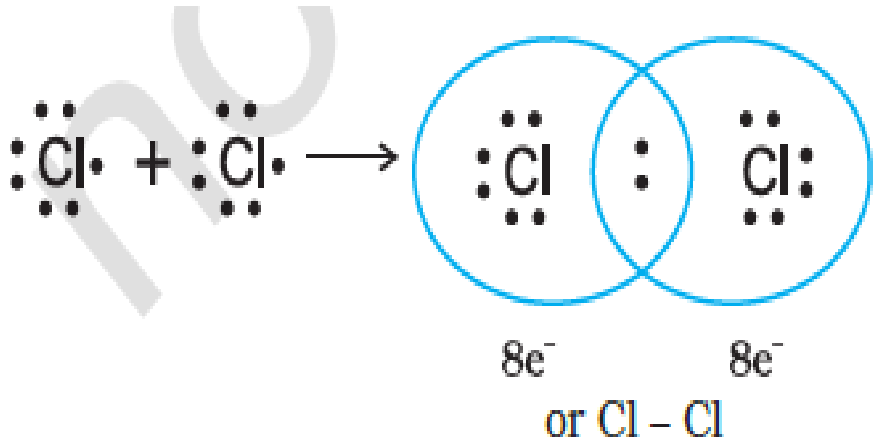


Figure 19.5
Electronic charge density in a [100] plane of NaCl containing the ions, as inferred from X-ray diffraction data. The numbers give the values of the density along lines of constant density, in units of electrons per cubic angstrom. The lines perpendicular to the constant density curves are error bars. (After G. Schoknecht, *Z. Naturforschung* 12, 983 (1957).)

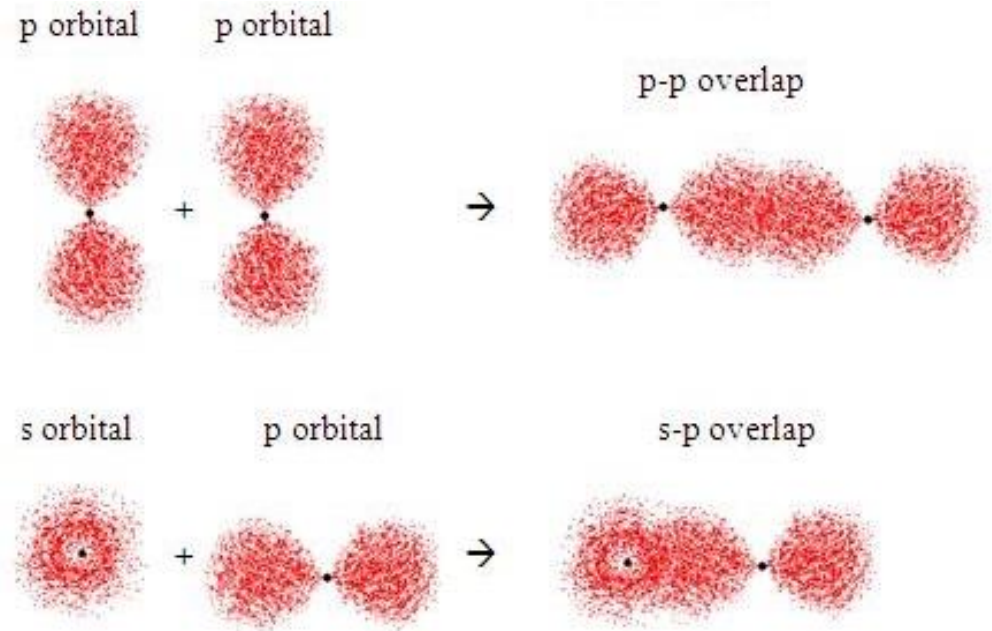


ClNa

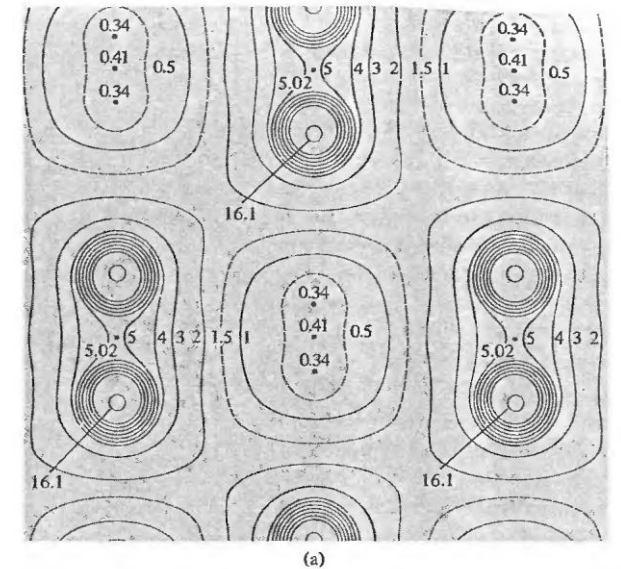
Uniones covalentes



Covalent bond between two Cl atoms



Densidad electronica en diamante



Uniones metálicas

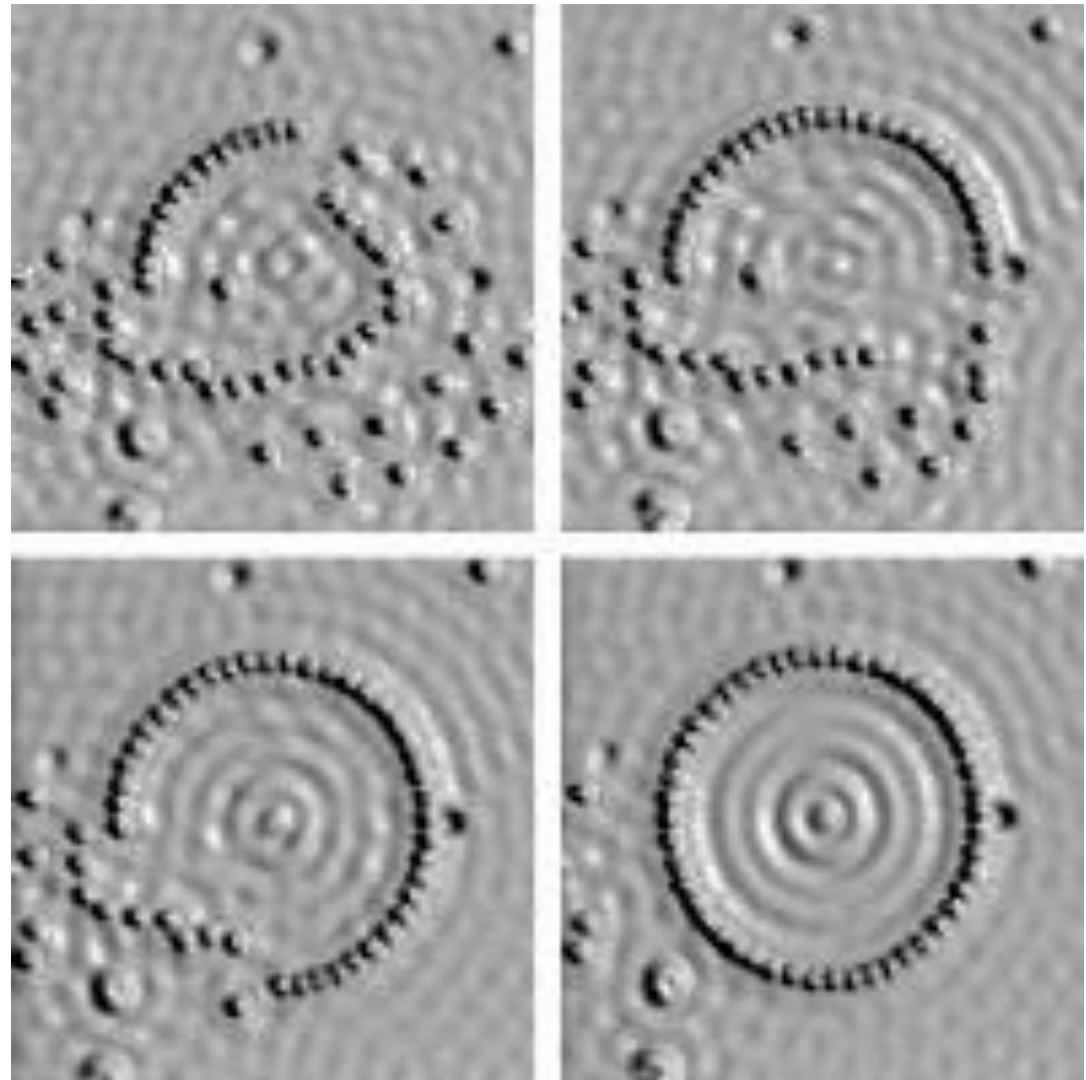


Imagen STM - IBM - Almaden USA

Algunas propiedades de la red de iones no se pueden describir con una red fija!!

