July 15, 17:00-18:00
Online

Seminar

High pressure electrides: a chemical and physical theory

Roald Hoffmann

Doctor of Chemistry, Professor at Cornell University, 1981 Nobel Prize Laureate in Chemistry

Speaker introduction

Roald Hoffmann was born in 1937 in Złoczów, then Poland. He came to the US in 1949, and has long been at Cornell, active as a theoretical chemist. In chemistry he has taught his colleagues how to think about electrons influencing structure and reactivity, and won most of the honors of his profession.
Hoffmann is also a writer, carving out his own land between poetry, philosophy, and science. He has published six books of non-fiction, three plays, and seven volumes of poetry, including two book length selections of his poems in Spanish and Russian translations.

Invited by Dr. Christian Tantardini, Research Scientist at CEST.

Seminar abstract

Electrides, in which electrons occupy interstitial regions in the crystal and behave as anions, have been known for some time, in liquid and solid phases. They also appear as new phases for many elements (and compounds) under high pressure. In work led by Mao-Sheng Miao we describe high pressure electrides (HPEs)
by treating electrons in the interstitial sites as filling the quantized orbitals of the space enclosed by the surrounding atom cores, generating what we call an interstitial quasi-atom, ISQ. With increasing pressure, the energies of the valence orbitals of atoms increase more significantly than the ISQ levels, orthogonality to the atom cores effectively being responsible. At a high enough pressure, which depends on the element and its orbitals, electron transfer to the interstitial space and the formation of an HPE may ensue. By using a He lattice model to compress atoms and an interstitial space, we are able to semi-quantitatively explain and predict the propensity of various elements to form HPEs. The slopes in energy of various orbitals with pressure (s>p>d for a given principal quantum number) are essential for identifying trends across the entire periodic table. ISQs can behave as radicals or anions, and in certain circumstances can form quasimolecules. We indicate evidence for such a system in Li under pressure.

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