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Direct Band Gap with Allotropes of Silicon Zeolite

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Description

The ability of some chemical elements or allotropes of the elements, to exist in two or more distinct forms in the same physical state is known as allotropy. Different structural alterations of an element are known as allotropes: The way the elements atoms are linked together is different. Compounds are not included in the definition of allotropy; only elements are included. Polymorphism is the more general term for any compound, although it is typically restricted to solids like crystals. Only distinct forms of an element within the same physical phase the state of matter are referred to as allotropes. Allotropy would not only be demonstrated by the differences in these states of matter. Polymorphs and phases of the element are common names for allotropes of chemical elements. Allotropes are distinct structural forms of the same element that can have very distinct chemical behaviors and physical properties. The same forces that affect other structures pressure, light, and temperature cause the transition between allotropic forms. The phenomenon of the same substance having distinct crystalline forms is known as polymorphism. Polymorphs are such forms or shapes. Crystalline materials are the only ones that can experience this phenomenon.

Silica Zeolites

Finding silicon allotropes with a high mobility, direct band gap, and high light absorption to replace conventional diamond silicon is a significant challenge in the fields of semiconductor and optoelectronic devices initio calculations were used to select fifteen silicon allotropes from hundreds of zeolite framework silicon allotropes with a direct band gap of 0.47–1.66 eV. Numerous allotropes are promising candidates for use in photovoltaic applications due to their easy doping, low carrier effective mass, and high solar spectrum absorption in comparison to diamond silicon. Zeolites are microporous, crystalline aluminosilicate materials that are frequently utilized as commercial adsorbents and catalysts. In a solution of contacting electrolytes, these positive ions can be exchanged for others. Zeolites mostly consist of silicon, aluminum, and oxygen. A wide range of cations, including Na^+, K^+, Ca^{2+}, Mg^{2+} and others can be accommodated in the microporous structures of zeolites. In a contacting electrolyte solution, these positive ions are frequently loosely held and readily exchangeable for other ions. High silica zeolites are zeolites with Si/Al ratios greater than or equal to three. These zeolites are rarely found in nature and are manufactured in industry. Due to the substantial contribution of covalent bonding, they exhibit high chemical and physical stability. They are suitable for the adsorption of sticky, hydrophobic molecules like hydrocarbons due to their excellent hydrophobicity. In addition, high silica zeolites, in contrast to natural zeolites, can exchange H^+ and are utilized as solid acid catalysts. High silica zeolites are used in acid catalysis procedures like fluid catalytic cracking in the petrochemical industry because the acidity is strong enough to protonate hydrocarbons.

Despite the fact that semiconductors of the second and third generations have been proposed for quite some time, silicon still has a wide range of applications in the fields of photovoltaic power and microelectronics due to its abundance of mature technology. However, its potential for photovoltaic applications in the future is limited by the indirect band gap and low solar absorptivity. Although numerous new materials have been proposed to replace silicon, their industry level application is constrained by their low natural reserves and high synthetic costs. Researchers have identified a wide range of potential silicon allotropes after conducting extensive research on dynamic stability, thermodynamic stability, and mechanical stability. The upper right provides an illustration of the notation for the ring structure of zeolite and other silicate materials. A four membered oxygen ring is formed when oxygen atoms are joined together. In point of fact, this kind of ring substructure is known as a four membered ring. The most common representation of the frameworks topology, which depicts a four ring composed of Si atoms connected to one another.

Zeolite Framework

A semiconductors band gap can be either a direct band gap or an indirect band gap in semiconductor. If the crystal momentum of electrons and holes is the same in both the conduction band and the valence band, the band gap is said to be direct. A photon cannot be released from an indirect gap because the electron must first move through an intermediate state before transferring momentum to the crystal lattice. To satisfy conservation of energy and crystal momentum, interactions between electrons, holes, photons and other particles are required. Near a semiconductor band gap, a photon with energy has almost no momentum. Radiative recombination, in which an electron in the conduction band destroys a hole in the valence band, releases excess energy as a photon, is one important process. Silicons allotropes are structurally distinct varieties. Silicon that is crystal clear has a grayish color and a metallic luster. Doping elements of crystalline silicon include boron, gallium, germanium, phosphorus, and arsenic. Solid state electronic devices like computer chips, rectifiers, and solar cells make use of doped silicon. Zeolite framework allotropes mechanical properties and mechanical stability were also thoroughly examined. Diamond silicon is examined in the same way for comparison. The fact that the stiffness matrix has a positive definite value indicates that all of these silicon allotropes in the zeolite framework are mechanically stable. The majority of sunlight consists of visible light, with a small amount of infrared and ultraviolet light also present. The photon absorption in the infrared and visible ranges of these zeolite framework silicon allotropes is significantly higher than that of diamond silicon. However, it does much better at absorbing visible and infrared light than other allotropes, and this is in a region that is perfectly compatible with the solar spectrum. Absorption of electromagnetic radiation is the process by which matter, typically electrons bound in atoms, absorbs photons energy and converts it into the absorbers own internal energy. Due to their direct band gap, the predicted novel silicon allotropes all have higher photon absorption across the solar spectrum. Zeolite framework silicons direct band gap, low carrier effective mass and high photon absorption point to its potential as a replacement for diamond silicon in thin film solar cell applications. Doping guest atoms will give the zeolite framework silicon family more possibilities because of the large voids in the zeolite framework.