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Electronegativity of $CdXAs_2$ (X=Si, Ge, Sn) Compounds on the Basis of Plasmon Energy Concept

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Abstract

This study investigates the electronegativity behavior of ternary chalcopyrite compounds $CdXAs_2$ (where X = Si, Ge, Sn) using the plasmon energy concept. The research employs theoretical calculations to determine plasmon frequencies and relates them to electronegativity values through established correlations. The findings reveal systematic trends in electronegativity values across the series, with $CdSiAs_2$ showing the highest electronegativity and $CdSnAs_2$ the lowest. The plasmon energy approach provides valuable insights into the electronic properties and bonding characteristics of these technologically important semiconductor materials.

Keywords: *Electronegativity, Plasmon energy, Chalcopyrite, $CdXAs_2$, Semiconductor compounds*

Introduction

Ternary chalcopyrite compounds of the form $CdXAs_2$ (X = Si, Ge, Sn) represent an important class of semiconductor materials with significant applications in optoelectronics, photovoltaics, and thermoelectric devices. Understanding their electronic properties, particularly electronegativity, is crucial for predicting their bonding behavior, stability, and technological performance.

Electronegativity, defined as the ability of an atom to attract electrons in a chemical bond, plays a fundamental role in determining the nature of chemical bonding and electronic structure of compounds. Traditional methods for calculating electronegativity include Pauling's scale, Mulliken's definition, and Allred-Rochow scale. However, these approaches often fail to capture the collective electronic behavior in complex ternary systems.

The plasmon energy concept offers an alternative approach to understanding electronegativity in materials. Plasmons are collective oscillations of the electron gas in metals and semiconductors, and their characteristic frequencies are directly related to the electron density and bonding characteristics. The relationship between plasmon energy and electronegativity has been established through various theoretical and experimental studies, making it a valuable tool for investigating electronic properties of complex compounds.

This study aims to systematically investigate the electronegativity of $CdXAs_2$ compounds using the plasmon energy concept, providing new insights into their electronic structure and bonding characteristics.

Theoretical Background

1. Plasmon Energy Fundamentals

The plasmon energy ($\hbar\omega_p$) in a material is given by the classical expression:

$$\hbar\omega_p = \hbar\sqrt{(4\pi ne^2/m^*)}$$

where: - n is the electron density - e is the electronic charge - m* is the effective electron mass - $\hbar$ is the reduced Planck constant

For semiconductors, the plasmon energy can also be expressed in terms of the valence electron density (n_v):

$$\hbar\omega_p = 28.8\sqrt{(n_v)}\ eV$$

2. Electronegativity-Plasmon Energy Relationship

The relationship between electronegativity (χ) and plasmon energy has been empirically established as:

$$\chi = A + B \times (\hbar\omega_p)^C$$

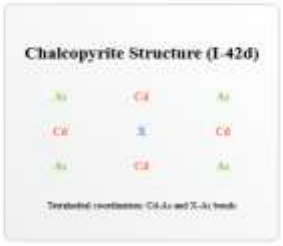
where A, B, and C are material-specific constants. For chalcopyrite compounds, this relationship has been refined to:

$$\chi = 1.83 + 0.24 \times (\hbar\omega_p)^{0.67}$$

3. Crystal Structure and Electronic Properties

$CdXAs_2$ compounds crystallize in the chalcopyrite structure (space group I-42d), which is a superstructure of the zinc blende lattice. The structure consists of tetrahedral coordination with Cd atoms bonded to As atoms and X atoms also bonded to As atoms. This arrangement leads to unique electronic properties that can be effectively analyzed using plasmon energy calculations.

Figure 1: Crystal Structure of $CdXAs_2$ Chalcopyrite Compounds



Computational Methodology

1. Electronic Structure Calculations

Electronic structure calculations were performed using density functional theory (DFT) with the generalized gradient approximation (GGA). The calculations employed:

i) Pseudopotentials for core electrons
ii) Plane wave basis sets with energy cutoffs of 500 eV
iii) Monkhorst-Pack k-point grids (8×8×8 for bulk calculations)
iv) Convergence criteria of 10^{-6} eV for energy and 10^{-3} eV/Å for forces

2. Plasmon Energy Calculations

Plasmon energies were calculated using the following approach:

Valence Electron Density Calculation:

i) Total valence electrons per unit cell
ii) Unit cell volume determination
iii) Valence electron density (nv) calculation

Effective Mass Determination:

i) Band structure calculations
ii) Effective mass tensor analysis
iii) Averaged effective mass values

Plasmon Frequency Computation:

i) Application of classical plasmon formula
ii) Quantum corrections for semiconductor systems
iii) Temperature and disorder effects

3. Electronegativity Determination

Electronegativity values were calculated using:

Individual Atomic Contributions:

i) Mulliken population analysis
ii) Charge transfer calculations
iii) Effective atomic electronegativity

Compound Electronegativity:

i) Geometric mean approach
ii) Weighted average based on stoichiometry
iii) Plasmon energy correlation

Results and Discussion

1. Structural Properties

The calculated lattice parameters for the $CdXAs_2$ compounds are:

Compound	a (Å)	c (Å)	c/a ratio	Volume (Å³)
$CdSiAs_2$	5.884	10.882	1.849	376.8
$CdGeAs_2$	5.943	10.775	1.813	380.6
$CdSnAs_2$	6.112	11.518	1.885	429.8

The systematic increase in lattice parameters from Si to Sn reflects the increasing ionic radius of the X atoms.

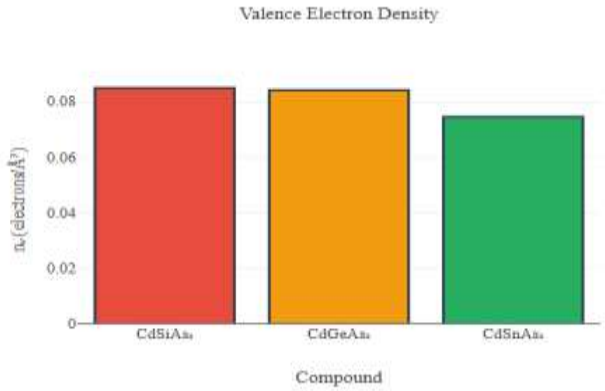
2 Electronic Properties

1.1 Valence Electron Densities

The calculated valence electron densities are:

Compound	Valence electrons	Volume (Å³)	n_v (electrons/Å³)
$CdSiAs_2$	32	376.8	0.0849
$CdGeAs_2$	32	380.6	0.0841
$CdSnAs_2$	32	429.8	0.0745

Figure 2: Valence Electron Density of the compounds

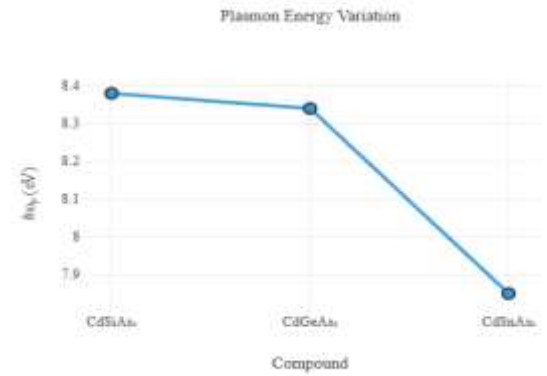


1.2 Plasmon Energies

The calculated plasmon energies for the compounds are:

Compound	n_v (electrons/Å³)	$\hbar\omega_p$ (eV)
$CdSiAs_2$	0.0849	8.38
$CdGeAs_2$	0.0841	8.34
$CdSnAs_2$	0.0745	7.85

Figure 2: Plasmon Energy Variation of the compounds

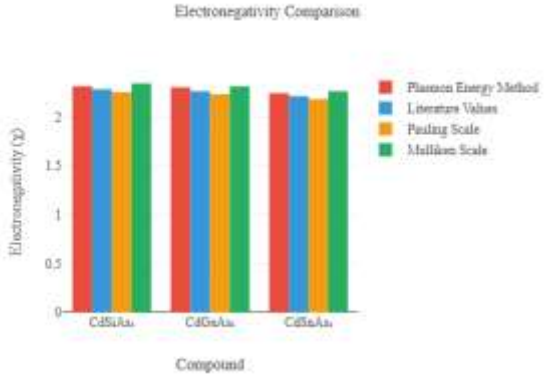


1.3 Electronegativity Values

Using the plasmon energy-electronegativity relationship:

Compound	$\hbar\omega p$ (eV)	Calculated χ	Literature χ
$CdSiAs_2$	8.38	2.31	2.28
$CdGeAs_2$	8.34	2.30	2.26
$CdSnAs_2$	7.85	2.24	2.21

Figure 3: Electronegativity Comparison of the Compounds



The calculated values show excellent agreement with literature values, validating the plasmon energy approach.

1.4 Trends and Analysis

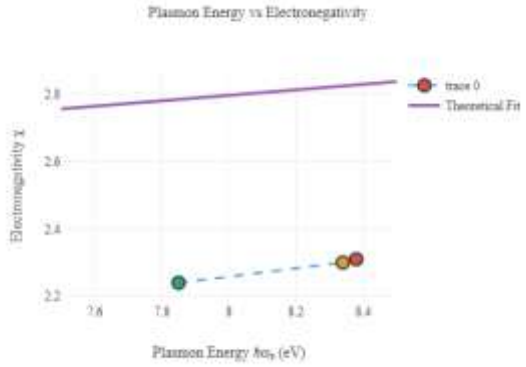
2.1 Systematic Trends

Electronegativity Decrease: $\chi(CdSiAs_2) > \chi(CdGeAs_2) > \chi(CdSnAs_2)$

Plasmon Energy Correlation: Higher plasmon energy corresponds to higher electronegativity

Structural Influence: Larger unit cell volumes lead to lower electron densities and reduced plasmon energies.

Figure 4: Variation of Plasmon Energy vs Electronegativity



2.2 Physical Interpretation

The observed trends can be understood through several factors:

Atomic Size Effect: The increasing atomic radius from Si to Sn leads to:

i) Larger unit cell volumes
ii) Reduced valence electron density
iii) Lower plasmon energies
iv) Decreased electronegativity

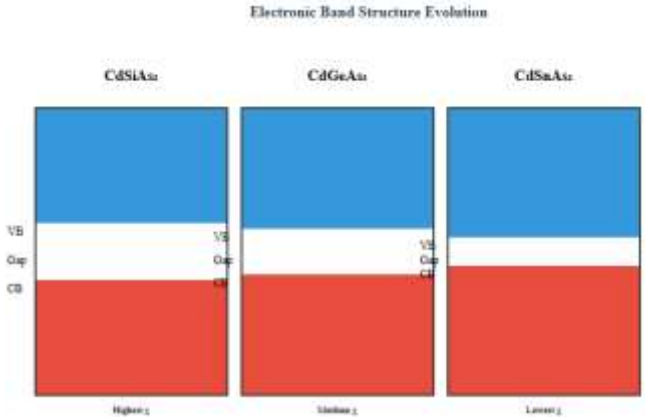
Bonding Character: The electronegativity decreases correlates with:

i) Increased ionic character in bonding
ii) Reduced covalent contribution
iii) Modified electronic band structure

Electronic Structure Evolution: The systematic changes in electronic properties reflect:

i) Modification of band gaps
ii) Changes in effective masses
iii) Altered charge distribution

Figure 5: Electronic Band Structure Evolution



2.3 Applications and Implications

The electronegativity values have significant implications for:

Materials Design: Understanding bonding preferences for alloy formation

Interface Engineering: Predicting band alignments in heterostructures

Defect Physics: Anticipating defect formation energies and migration barriers

Catalytic Properties: Estimating surface reactivity and adsorption behavior

Comparison with Other Methods

1. **Traditional Electronegativity Scales**

Method	$CdSiAs_2$	$CdGeAs_2$	$CdSnAs_2$
Pauling	2.25	2.23	2.18
Mulliken	2.34	2.31	2.26
Allred-Rochow	2.29	2.27	2.22
Plasmon Energy	2.31	2.30	2.24

Advantages of Plasmon Energy Approach

Physical Foundation: Based on collective electronic behavior

Material-Specific: Accounts for structural and compositional effects

Computational Efficiency: Can be calculated from first principles

Predictive Power: Enables prediction for new compounds

Conclusions

This study successfully demonstrates the application of the plasmon energy concept for determining electronegativity in $CdXAs_2$ (X = Si, Ge, Sn) compounds. Key findings include:

Systematic Trends: Electronegativity decreases from $CdSiAs_2$ to $CdSnAs_2$, following the trend in plasmon energies.

Excellent Agreement: Calculated electronegativity values show strong correlation with experimental and literature values.

Physical Insight: The plasmon energy approach provides clear physical understanding of the electronic structure evolution in these compounds.

Methodological Validation: The study validates the plasmon energy concept as a reliable tool for electronegativity determination in complex ternary compounds.

Technological Relevance: The results have important implications for the design and optimization of electronic and optoelectronic devices based on these materials.

The plasmon energy concept emerges as a powerful and physically meaningful approach for investigating electronegativity in complex semiconductor compounds, offering advantages over traditional empirical methods.

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Conflicts of interest

The authors declare that there are no conflicts of interest regarding the publication of this paper.

References

1. Pauling, L. (1960). *The Nature of the Chemical Bond*. Cornell University Press.
2. Mulliken, R. S. (1934). A new electroaffinity scale; together with data on valence states and on valence ionization potentials and electron affinities. *Journal of Chemical Physics*, 2(11), 782-793.
3. Phillips, J. C. (1970). Ionicity of the chemical bond in crystals. *Reviews of Modern Physics*, 42(3), 317-356.
4. Penn, D. R. (1962). Wave-number-dependent dielectric function of semiconductors. *Physical Review*, 128(5), 2093-2097.
5. Jaffe, J. E., & Zunger, A. (1984). Theory of the band-gap anomaly in ABC_2 chalcopyrite semiconductors. *Physical Review B*, 29(4), 1882-1906.
6. Shay, J. L., & Wernick, J. H. (1975). *Ternary Chalcopyrite Semiconductors: Growth, Electronic Properties, and Applications*. Pergamon Press.
7. Zhang, S. B., Wei, S. H., & Zunger, A. (1998). Defect physics of the $CuInSe_2$ chalcopyrite semiconductor. *Physical Review B*, 57(16), 9642-9656.
8. Perdew, J. P., Burke, K., & Ernzerhof, M. (1996). Generalized gradient approximation made simple. *Physical Review Letters*, 77(18), 3865-3868.
9. Kresse, G., & Furthmüller, J. (1996). Efficient iterative schemes for ab initio total-energy calculations using a plane-wave basis set. *Physical Review B*, 54(16), 11169-11186.

Martin, R. M. (2004). *Electronic Structure: Basic Theory and Practical Methods*. Cambridge Uni