CdTe is a II–VI semiconductor material with excellent characteristics and has demonstrated promising potential for application in the photovoltaic field. The electronic properties of Cd$_{43}$Te$_{28}$ with microporous structures are investigated based on density functional theory. The newly established binding-energy and bond-charge model is used to convert the value of Hamiltonian into bonding values. A method is provided for describing topological chemical bonds by atomic coordinates and wave phases. The dynamic process of the wave function with time and the magic cube matrix are also discussed. This study provides an innovative method and technology for the accurate analysis of the topological bonding and electronic properties of microporous semiconductor materials.

1. Introduction

Microporous materials are solids that involve regular pores or voids that are less than 2 nm in diameter.\textsuperscript{[1]} Metal–organic frameworks and zeolite are important components of the microporous material category. Most of the microporous materials are composed of connected TO$_4$ tetrahedrons (where T = tetrahedral atoms, such as Al, P, Si, etc.), wherein each oxygen atom is shared between two ring tetrahedrons, thus forming a framework with an O/T ratio of 2.\textsuperscript{[2–3]} These tetrahedrons are connected in such a way that regular pores and channels are formed in the material; therefore, a large portion of the material (up to 50% in some cases) is a real “space.” Pore systems of 1, 2, or 3D are formed inside the microporous material, and different molecules can be separated according to the geometric shapes of the microporous material. The geometric shape of the microporous material is determined by the size and uniformity of the pores, which is termed “shape selectivity.” By controlling the shape selectivity, specific reactant molecules enter the microporous material, and the molecules that can be passed into or form in the material are restricted (reactant selectivity).\textsuperscript{[4]} Similarly, specific products can be removed from materials (product selectivity), and transition states can be formed by specific products in the materials (transition state selectivity) based on this property. With the discovery and development of new types of materials, the applications, properties, and modifications related to microporous materials have become the focus of scientific research. The increased impetus of the rate of research is due to the excellent performance of microporous materials.

Recently, II–VI semiconductor compounds and alloys that are based on Cd have received extensive attention because of their applications in photovoltaic devices.\textsuperscript{[5–7]} Cadmium telluride (CdTe) is a p-type semiconductor with a high absorption rate and wide bandgap. Thus, it can be used as an effective material in solar thin-film cells, as it exhibits satisfactory efficiency and is cost effective. The working efficiency of the solar thin-film cells that comprises CdTe can be greater than 22%\textsuperscript{[8]} The wide bandgap and high absorption rate of CdTe meet the requirements of solar thin-film cells. The absorption edge of CdTe is sharp due to the direct bandgap,\textsuperscript{[9]} and over 90% of the incident light can be absorbed by the material. The maximum photocurrent of the CdTe thin-film solar cells reaches 30.5 mA cm$^{-2}$ under an irradiation of 100 mW cm$^{-2}$ optical power density, and the value of the theoretical maximum efficiency exceeds 27%.\textsuperscript{[10]} Due to its vast application prospects, the CdTe semiconductor reached a level comparable with that of single-crystal materials that are more complex.\textsuperscript{[11]}

Numerous theoretical and experimental studies have been performed on CdTe semiconductor materials.\textsuperscript{[12–14]} Herein, we report the CdTe semiconductor materials that have a microporous structure. The geometric structure of Cd$_{43}$Te$_{28}$ microporous material is obtained by self-assembly of nanocluster structure. The geometric structure of different types of Cd$_{43}$Te$_{28}$ has been optimized using density functional theory (DFT) calculations. Furthermore, the bonding and electronic properties of Cd$_{43}$Te$_{28}$ semiconductor microporous materials have been studied. The newly established binding-energy and bond-charge (BBC) model has been used to convert the value of Hamiltonian into the values of nonbonding, bonding, and antibonding, and the relationship between the relevant physical and chemical performance parameters of the materials and their chemical bonding was ascertained.\textsuperscript{[15–17]}

The BBC model is quantified by chemical bonds by binding energy shift and deformation charge density. For the binding energy shift, we use the central field approximation\textsuperscript{[18]} and tight binding (TB) model,\textsuperscript{[19]} which can get the relationship between

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the energy shift and Hamiltonian. For the bond-charge model, we use the second-order term of energy expansion and use deformation charge density to calculate bonding states. For the topological structure, we use the fiber worm principle of quantum mechanics and the geometric phase of Berry.\cite{20}

In theory, by regulating the unique microporous structure and bonding performance of the semiconductor, the photoelectric properties of Cd_{43}Te_{28} can be improved markedly.

2. Model and Methods

2.1. Density Functional Theory Calculations

All the structural relaxation and electronic properties of Cd_{43}Te_{28} microporous materials were investigated with Cambridge Sequential Total Energy Package (CASTEP),\cite{21} which used DFT with a planewave pseudopotential. This analysis was focused on analyzing the atomic structure, energetics, and electronic properties of Cd_{43}Te_{28} microporous materials. We used local density approximation (LDA) and Perdew–Burke–Ernzerhof (PBE) to describe the electron exchange and correlation potential.\cite{22,24}

The cutoff energy of the planewave basis set was 400 eV. The k-point grids were 3 × 3 × 3, as shown in Table 1. In the calculations, all the atoms were completely relaxed such that the energy converged to 10^{-6} and the force on each atom converged to < 0.01 eV Å^{-1}.

2.2. BBC Model

The TB model leads to the Hamiltonian formulas:\cite{25,28}

\[
\begin{align}
H &= \frac{-\hbar^2 \nabla^2}{2m} + V_0(\vec{r}) + V_{\text{c}}(\vec{r})(1 + \Delta_{\text{HI}}) \\
V_{\text{c}}(\vec{r}) &= V_{\text{c}}(\vec{r})(1 + \Delta_{\text{HI}}) = \gamma V_{\text{c}}(\vec{r}) \\
E_0(0) &= -\langle \phi_0(\vec{r}) | \frac{-\hbar^2 \nabla^2}{2m} + V_0(\vec{r}) | \phi_0(\vec{r}) \rangle \\
E_{\text{c}}(x) &= E_{\text{c}}(0) = -\langle \phi(\vec{r}) | V_{\text{c}}(\vec{r}) | \phi(\vec{r}) \rangle \\
&= \gamma \alpha_v \left( 1 + \frac{\sum |\phi_i(\vec{r})|}{\alpha_v} \right) \\
&\approx \gamma \alpha_v \alpha E_{\text{c}} \\
\left\{ \begin{array}{c}
\alpha_v = -\langle \phi_v(\vec{r}) | V_{\text{c}}(\vec{r}) | \phi_v(\vec{r}) \rangle \\
\beta_v = -\langle \phi_v(\vec{r}) | V_{\text{c}}(\vec{r}) | \phi_v(\vec{r}) \rangle \\
\end{array} \right.
\end{align}
\]

(1)

(2)

(3)

where $E_c(i)$ is the i-th energy level of a crystal and $E_c(0)$ is the i-th energy level of an isolated atom. $V_c(\vec{r})$ and $V_{\text{c}}(\vec{r})$ are the potential energies of the atom and crystal, respectively; $\phi_v(\vec{r})$ represents an atomic orbital of the i-th energy level; $E_v$ represents the single-bond energy. Both $\alpha_v$ and $\beta_v$ in Equation (2) contribute to the energy band width. However, the energy band of the core energy level is determined by $\alpha_v$, because $\beta_v$ is very small in the local energy band of the core energy level, the term $\sum |\phi_v(\vec{r})| \beta_v \ll 1$.

The wave function is $\psi_\ell(\vec{r}) = \frac{1}{\sqrt{N}} \sum e^{i \vec{k} \cdot \vec{R}_j} \phi(\vec{r} - \vec{R}_j)$. The form of the periodic factor $f(\vec{k})$ is $e^{i \vec{k} \cdot \vec{R}}$, where $k$ represents the wave vector. The quantity $\beta$ depends on the overlap between the orbitals centered at two neighboring atoms; $\vec{r}$ represents the electron coordinates and $\vec{R}$ represents the nuclei coordinates.

Considering the time-dependent potential function

\[
\begin{align}
&\left\{ \begin{array}{c}
V_{\text{c}}(\vec{r}, t) = (1 + f(\vec{k})) V_0(\vec{r}) \\
\zeta(f(t)) = F(s) = \int_{-\infty}^{+\infty} f(t) e^{-\gamma t} dt \\
f(t) = \zeta^{-1}(F(s)), \quad \hat{S}_t = e^{-i\hat{F}/\hbar} = e^{-i\hat{F}t} \\
\end{array} \right. \\
&\left\{ \begin{array}{c}
V_{\text{c}}(\vec{r}, t) = V_{\text{c}}(\vec{r}) (1 + \Delta_{\text{HI}}) = \gamma V_{\text{c}}(\vec{r}) \\
V_{\text{c}}(\vec{r}) = -\frac{1}{4\pi \varepsilon_0} \int \frac{Z^2 e^2}{|\vec{r} - \vec{R}|} \\
&= \sum_{i,j,k} \frac{1}{4\pi \varepsilon_0} \frac{Z^2 e^2}{|\vec{r} - \vec{R}_i|} \end{array} \right. \\
&\left\{ \begin{array}{c}
V_{\text{c}}(\vec{r}, t) = V_{\text{c}}(\vec{r}) (1 + \Delta_{\text{HI}}) = \gamma V_{\text{c}}(\vec{r}) \\

\end{array} \right.
\end{align}
\]

(4)

(5)

The core electrons will not only be attracted by the nuclear charge, but also be excluded by other electrons. The repulsive effect of electrons will reduce the attractive effect of the nucleus. The effective positive charge of the ion is $Z' = Z - \sigma$, considering the charge-shielding effect ($\sigma$), where $Z$ is the nuclear charge.

Table 2. Laplace transform formula.

| Primitive function | Laplace transform | Convergence region |
|--------------------|------------------|--------------------|
| $f(t)$ | $F(s) = \zeta^{-1}(F(s))$ | $\beta(t)$ | $1$ | $\infty > s > -\infty$ |
| $i$ | $\frac{1}{\sqrt{s}}$ | $s > 0$ |
| $e^{-at}$ | $\frac{1}{\sqrt{a}}$ | $s > -a$ |
| $\sin(at)$ | $\frac{a}{\sqrt{s^2 + a^2}}$ | $s > 0$ |
| $\cos(at)$ | $\frac{a}{\sqrt{s^2 + a^2}}$ | $s > 0$ |
| $\sinh(at)$ | $\frac{a}{\sqrt{s^2 - a^2}}$ | $s > a$ |
| $\cosh(at)$ | $\frac{a}{\sqrt{s^2 - a^2}}$ | $s > a$ |
| $e^{at} \sin(bt)$ | $\frac{b}{\sqrt{s^2 + b^2}}$ | $s > a$ |
| $e^{at} \cos(bt)$ | $\frac{b}{\sqrt{s^2 + b^2}}$ | $s > a > |b|$ |
| $e^{at} \sinh(bt)$ | $\frac{b}{\sqrt{s^2 - b^2}}$ | $s > a > |b|$ |

Table 1. Lattice parameters cutoff and k-point of Cd_{43}Te_{28} microporous materials.

| Structure | Cutoff | k-point | Angles | Lattice parameters |
|-----------|--------|---------|--------|-------------------|
| Cutoff | $\alpha$ | $\beta$ | $\gamma$ | $a$ | $b$ | $c$ | $\alpha$ | $\beta$ | $\gamma$ |
| Cd_{43}Te_{28} | 400 eV | $3 \times 3 \times 3$ | 90.00° | 90.00° | 90.00° | 16.118 | 16.118 | 16.118 |\[Image\]
\( \sigma = \frac{|\vec{r}_i - \vec{R}_j|}{|\vec{r}_i - \vec{r}_j|} \) can be written as a Hamiltonian containing electron interaction terms. However, considering the repulsion of electrons, the effective positive charge number \( Z' \) of the ion can be varied, as shown in Figure 1. When the valence electron density decreases, the shielding effect will be weakened and the binding energy of the core electrons will increase. On the contrary, the binding energy will decrease.

\[
\Delta E_v(x) = E_v(x) - E_v(0) = -\langle \phi_v(r) | V_c(\vec{r}) (1 + \Delta \delta) | \phi_v(r) \rangle \\
= -\langle \phi_v(r) | V_c(\vec{r}) | \phi_v(r) \rangle - \langle \phi_v(r) | \delta \phi_v(r) \rangle
\]

From Equation (2) and (5), we obtain Equation (7)

\[
\Delta E_v(B) = E_v(x) - E_v(B) = -\langle \phi_v(r) | V_c(\vec{r}) | \delta \phi_v(r) \rangle
\]

The energy-level shifts in an external field obtained from Equation (5)–(7) are as follows (where \( Z \) represents the atomic charge number, \( \gamma = 1 + \Delta \delta \) are the binding energy ratio and relative binding energy ratio \( \delta \gamma \), respectively, and \( B \) indicates the bulk atoms. \( \varepsilon_0 \) is the dielectric constant of the vacuum):

\[
\begin{align*}
\delta \gamma &= -1 \quad \text{(Antibonding)} \quad \Delta E_v(x) = \Delta E_v(0) = 0 \quad \text{(isolated atom, neutral atom)} \\
\delta \gamma &= 0 \quad \text{(Bonding)} \quad \Delta E_v(x) = \Delta E_v(B) = -\left( -\sum_{l, l' \neq 0} \langle \phi_l(r) | \frac{1}{4 \pi \varepsilon_0 |\vec{r} - \vec{R}_l|} | \phi_l(r) \rangle \right) > 0 \quad \text{(bulk atoms, core level loses electrons)} \\
\delta \gamma &= 0 \quad \text{(Bonding)} \quad \Delta E_v(x) = -\left( -\langle \phi_v(r) | \sum_{l, l' \neq 0} \frac{(1 + \Delta \delta)}{4 \pi \varepsilon_0 |\vec{r} - \vec{R}_l|} | \phi_v(r) \rangle \right) > 0 \quad \text{(potential well becomes deeper)} \\
1 > \Delta \gamma > 0 \quad \text{(Bonding)} \quad \Delta E_v(x) = -\left( -\langle \phi_v(r) | \sum_{l, l' \neq 0} \frac{(1 \Delta \delta)}{4 \pi \varepsilon_0 |\vec{r} - \vec{R}_l|} | \phi_v(r) \rangle \right) > 0 \quad \text{(core level loses electrons)} \\
-1 < \Delta \gamma < 0 \quad \text{(Nonbonding)} \quad \Delta E_v(x) = -\left( -\sum_{l, l' \neq 0} \langle \phi_v(r) | \frac{(1 + \Delta \delta)}{4 \pi \varepsilon_0 |\vec{r} - \vec{R}_l|} | \phi_v(r) \rangle \right) < 0 \quad \text{(potential well becomes shallower or barrier potential)}
\end{align*}
\]

Equation (8) was obtained by calculating the external field-induced binding energy (BE) ratio, \( \gamma \), using the known reference values of \( \Delta E_v(x) = E_v(x) - E_v(B) \) and \( \Delta E_v(x) = E_v(x) - E_v(0) \) derived from X-ray photoelectron spectroscopy (XPS) analysis. Then, we obtain

\[
\gamma = \frac{E_v(x) - E_v(0)}{E_v(B) - E_v(0)} = \frac{Z_b - \sigma'}{Z_b} \left( \frac{Z_b - \sigma'}{Z_b} \right)^{-1} = \left( \frac{d_v}{d_b} \right)^{-m} = \frac{E_x}{E_b}
\]

\( \sigma' \) is the relative charge shielding factor. \( m \) is an indicator for the bond nature of a specific material. \( m \) is related to the charge shielding factor \( \sigma' \), \( m = 1 - \frac{\ln(\frac{Z_b - \sigma'}{Z_b})}{\ln(\frac{Z_b - \sigma}{Z_b})} \). The binding energy shifts in the BBC model are derived from the extended model of bond–order–length–strength (BOLS) theory. The difference is that we use the central force field method and considering the effect of electronic shielding, the DFT calculation data is basically consistent with the XPS experimental data. 

Equation (10) was obtained by considering the effect of the charge transfer of the bond–charge model.

\[
E[\rho_0 + \delta \rho] = E[\rho_0] + E'[\rho_0 + \delta \rho] + E^2[\rho_0, (\delta \rho)^2] \\
= \sum \langle \phi_i | -\frac{1}{2} \nabla^2 + V_{ext} \vec{r} | \phi_i \rangle \\
- \frac{1}{2} \int \int \frac{\rho_0(\vec{r}) \rho(\vec{r}')}{|\vec{r} - \vec{r}'|} d\vec{r} d\vec{r}' \\
- \int V_{XC}[\rho_0, \rho(\vec{r})] d\vec{r} + E^2[\rho_0] \\
+ \sum \int \overline{\epsilon_i} + \frac{1}{2} \int \int \frac{1}{|\vec{r} - \vec{r}'|} \delta \rho(\vec{r}) \delta \rho(\vec{r}') d\vec{r} d\vec{r}'
\]

\( \delta \rho = \rho - \rho_0 \) is the charge density gradient. \( \overline{\epsilon_i} \) is the average dielectric constant of the material. \( \rho_0(\vec{r}) \) is the total electronic charge density. \( \rho(\vec{r}) \) is the charge density of the core electrons. \( V_{XC} \) is the exchange correlation potential.
where $E^1[\rho_0]$ is termed the “repulsive energy” which determines the dispersion of the energy band. $V^{XC}$ and $E^{XC}$ are the potential and exchange correlation energies, respectively, and are typically fit from the DFT calculations. In the second term, $E^2[\rho_0 + \delta \rho]$, $\varepsilon_i$ indicates the ith electronic level and $f_i$ is the corresponding electronic occupation number. In the second term, $E^2[\rho_0, (\delta \rho)^2]$, $\rho_0(\vec{r})$ is the initial density function, and $\delta \rho(\vec{r})$ is the deformation density function. Therefore, Equation (11) was obtained.

$$\Delta V_{bc}(\vec{r} - \vec{r'}) = \frac{1}{8\pi\epsilon_0} \int d^3r \int d^3r' \frac{\delta \rho(\vec{r}) \delta \rho(\vec{r'})}{|\vec{r} - \vec{r'}|}$$

(11)

where $\Delta V_{bc}(\vec{r}_i)$ is the deformation charge of the bond energy. Additionally, the deformation density $\delta \rho$ satisfies the following relationship (Equation (12)).

$$\delta \rho_{\text{Hole-electron}} \leq \delta \rho_{\text{Antibonding-electron}} < \delta \rho_{\text{No charge transfer}} = 0 < \delta \rho_{\text{Nonbonding-electron}} \leq \delta \rho_{\text{Bonding-electron}}$$

(12)

For bonding (Equation (13))

$$\delta \rho_{\text{Hole-electron}}(\vec{r}) \delta \rho_{\text{Bonding-electron}}(\vec{r}) < 0 \quad \text{(Strong Bonding)}$$

(13)

For nonbonding or weak bonding (Equation (14))

$$\begin{cases}
\delta \rho_{\text{Hole-electron}}(\vec{r}) \delta \rho_{\text{Nonbonding-electron}}(\vec{r}) < 0 \\
(\text{Nonbonding or Weak Bonding}) \\
\delta \rho_{\text{Antibonding-electron}}(\vec{r}) \delta \rho_{\text{Bonding-electron}}(\vec{r}) < 0 \\
(\text{Nonbonding or Weak Bonding}) \\
\delta \rho_{\text{Antibonding-electron}}(\vec{r}) \delta \rho_{\text{Nonbonding-electron}}(\vec{r}) < 0 \\
(\text{Nonbonding}) 
\end{cases}$$

(14)

For antibonding (Equation (15))

$$\begin{cases}
\delta \rho_{\text{Nonbonding-electron}}(\vec{r}) \delta \rho_{\text{Bonding-electron}}(\vec{r}) > 0 \\
(\text{Antibonding}) \\
\delta \rho_{\text{Hole-electron}}(\vec{r}) \delta \rho_{\text{Antibonding-electron}}(\vec{r}) > 0 \\
(\text{Antibonding}) \\
\delta \rho_{\text{Hole-electron}}(\vec{r}) \delta \rho_{\text{Hole-electron}}(\vec{r}) > 0 \\
(\text{Antibonding}) \\
\delta \rho_{\text{Antibonding-electron}}(\vec{r}) \delta \rho_{\text{Antibonding-electron}}(\vec{r}) > 0 \\
(\text{Antibonding}) \\
\delta \rho_{\text{Nonbonding-electron}}(\vec{r}) \delta \rho_{\text{Nonbonding-electron}}(\vec{r}) > 0 \\
(\text{Antibonding}) \\
\delta \rho_{\text{Bonding-electron}}(\vec{r}) \delta \rho_{\text{Bonding-electron}}(\vec{r}) > 0 \\
(\text{Antibonding}) 
\end{cases}$$

(15)

It is noteworthy that the formation of the chemical bonds is related to the fluctuations in electron density. For the total deformation charge of the bond energy, we can write it as

$$\Delta V_{bc}(\vec{r} - \vec{r'}) = \frac{1}{N} \left( \sum_i V_{at}(\vec{r} - \vec{r'}) + \sum_j V_{rep}(\vec{r} - \vec{r'}) \right)$$

$$\Delta V_{bc}(\vec{r} - \vec{r'}) = \frac{1}{N} \left( \Delta V_{\text{Bonding}}(\vec{r} - \vec{r'}) + \Delta V_{\text{Nonbonding}}(\vec{r} - \vec{r'}) \right)$$

$$+ \Delta V_{\text{Antibonding}}(\vec{r} - \vec{r'}) \quad (N = i + j)$$

(16)

$V_{\text{rep}}(\vec{r} - \vec{r'})$ represents the bond energy of repulsion and $V_{\text{at}}(\vec{r} - \vec{r'})$ represents the bond energy of attraction.

Consider the influence of external field on deformation charge of the bond energy, we introduce the scale of bond energy

$$\Delta V_{bc}(\vec{r} - \vec{r'}) = \Delta V_{bc0}(\vec{r} - \vec{r'}) e^{-\lambda r}$$

(17)

$\lambda$ is the external field shielding parameter of bond energy deformation charge.

From the Hubbard model, we get

$$\hat{V}_{ee} = \frac{1}{2} \int d^3r \int d^3r' \alpha_\zeta(\vec{r}) \alpha_\zeta(\vec{r'}) V_{ee}(\vec{r} - \vec{r'}) \alpha_\zeta(\vec{r}) + \langle \vec{r'} \rangle \alpha_\zeta(\vec{r'})$$

$$= \frac{1}{2|\vec{r} - \vec{r'}|} \int d^3r \int d^3r' \rho(\vec{r}) \rho(\vec{r'})$$

(18)

where $\alpha_\zeta(\vec{r})$ and $\alpha_\zeta(\vec{r'})$ are annihilation and creation operators, respectively. For the sake of completeness, we endowed the electrons with a spin index, $\zeta = \uparrow / \downarrow$. The charge density is $\rho(\vec{r}) = \alpha_\uparrow(\vec{r}) \alpha_\downarrow(\vec{r})$. The quantity $V_{ee}(\vec{r} - \vec{r'}) = \frac{1}{2|\vec{r} - \vec{r'}|}$ is the potential of the electron, which induces a transformation

$$\alpha_\uparrow(\vec{r}) = \sum \psi_{\uparrow}(\vec{r}) a_{\uparrow}^\dagger$$

(19)

Inserting Equation (19) into (18) leads to the expansion

$$\hat{V}_{ee} = \sum_{ij} U_{ij} a_{\uparrow i}^\dagger a_{\downarrow j} + \sum_{i} \psi_{\uparrow i}(\vec{r})$$

where

$$U_{ij} = \frac{1}{2} \int d^3r \int d^3r' \psi_{\uparrow j}(\vec{r}) \psi_{\downarrow i}(\vec{r}) V_{ee}(\vec{r} - \vec{r'}) \psi_{\downarrow j}(\vec{r}) \psi_{\uparrow i}(\vec{r})$$

(20)

is the Coulomb interaction.

Therefore, the electron density fluctuations can also be represented by the Hubbard model.

$$\Delta V_{bc}(\vec{r} - \vec{r'}) = \pm \frac{1}{2} \int d^3r \int d^3r' \alpha_\zeta(\vec{r}) \alpha_\zeta(\vec{r'}) V_{ee}(\vec{r} - \vec{r'}) \alpha_\zeta(\vec{r'})$$

$$+ \langle \vec{r'} \rangle \alpha_\zeta(\vec{r'})$$

$$= \frac{1}{2|\vec{r} - \vec{r'}|} \int d^3r \int d^3r' \delta \rho(\vec{r}) \delta \rho(\vec{r'})$$

(21)

The deformation charge–bond energy $\Delta V_{bc}(\vec{r} - \vec{r'})$ is different from the Coulomb repulsion energy $\hat{V}_{ee}$. The deformation...
charge–bond energy considers the interaction between electrons and holes, and there are three cases of bonding, antibonding, and nonbonding. For the bond–charge model of BBC model, its source is the second-order term of energy expansion.

### 2.3. Time-Dependent First-Order Response Wave Function

For systems of linear differential equations with constant coefficients:

\[ x'(t) = Ax(t) \]  

\( A \) is a matrix. Column vector \( x \) is the physical quantity of first-order time response that can be derived, for example, wave function \( \varphi \), electric field \( E \), magnetic field \( B \), density \( \rho \), etc.

Consider homogeneous linear differential equations with constant coefficients of two variables:

\[
\begin{align*}
\frac{d}{dt} \begin{pmatrix} x_1(t) \\ x_2(t) \end{pmatrix} &= A \begin{pmatrix} x_1(t) \\ x_2(t) \end{pmatrix} \\
A &= \begin{pmatrix} c_{11} & c_{12} \\ c_{21} & c_{22} \end{pmatrix}
\end{align*}
\]  

(23)

Let \( \lambda_1 \) and \( \lambda_2 \) be the characteristic roots of coefficient matrix \( A \) of the Equation (23), then

(i) When \( c_{12} = 0, c_{11} = c_{22} \), the basic solution matrix of Equation (23) is

\[
\Phi(t) = \begin{pmatrix} e^{\lambda_1 t} & 0 \\ \frac{c_{11}}{c_{22}} e^{\lambda_1 t} & e^{\lambda_2 t} \end{pmatrix}
\]  

(24)

(ii) When \( c_{12} = 0, c_{11} \neq c_{22} \), the basic solution matrix of Equation (23) is

\[
\Phi(t) = \begin{pmatrix} e^{\lambda_1 t} & 0 \\ \frac{c_{11}}{c_{22}} e^{\lambda_1 t} - e^{\lambda_2 t} \end{pmatrix}
\]  

(25)

(iii) When \( c_{12} \neq 0 \), and \( \lambda_1, \lambda_2 \) are unequal real roots, the basic solution matrix of Equation (23) is

\[
\Phi(t) = \begin{pmatrix} e^{\lambda_1 t} & 0 \\ \frac{\lambda_1 - c_{11}}{c_{12}} e^{\lambda_1 t} - \frac{\lambda_2 - c_{11}}{c_{12}} e^{\lambda_2 t} \end{pmatrix}
\]  

(26)

(iv) When \( c_{12} \neq 0 \), and \( \lambda_1, \lambda_2 \) are equal real roots, the basic solution matrix of Equation (23) is

\[
\Phi(t) = \begin{pmatrix} e^{\lambda_1 t} & 0 \\ \frac{c_{11}}{c_{12}} e^{\lambda_1 t} - \frac{1 + (c_{11} - c_{11})^2}{c_{12}} e^{\lambda_1 t} \end{pmatrix}
\]  

(27)

(v) When \( c_{12} \neq 0 \), and \( \lambda_1, \lambda_2 \) are conjugate complex roots, the basic solution matrix of Equation (23) is

\[
\Phi(t) = \begin{pmatrix} e^{\alpha t} \cos \beta t & e^{\alpha t} \sin \beta t \\ e^{\alpha t} \sin \beta t & e^{\alpha t} \cos \beta t \end{pmatrix}
\]  

(28)

Consider wave function of \( sp \) equivalent hybridization

\[
\begin{align*}
\varphi_1 &= \sqrt{\frac{1}{2}} \varphi_s + \sqrt{\frac{1}{2}} \varphi_p \\
\varphi_2 &= \sqrt{\frac{1}{2}} \varphi_s - \sqrt{\frac{1}{2}} \varphi_p
\end{align*}
\]  

(29)

Then, matrix formation (29)

\[
\begin{pmatrix} \varphi_1(t) \\ \varphi_2(t) \end{pmatrix} = \begin{pmatrix} \sqrt{\frac{1}{2}} & \sqrt{\frac{1}{2}} \\ \sqrt{\frac{1}{2}} & -\sqrt{\frac{1}{2}} \end{pmatrix} \begin{pmatrix} \varphi_1(t) \\ \varphi_2(t) \end{pmatrix}
\]  

(30)

If the wave function obtained is a first-order response function with time, we have

\[
\Phi(t) = \begin{pmatrix} 1 - \sqrt{\frac{1}{2}} e^t & -1 + \sqrt{\frac{1}{2}} e^{-t} \\ \sqrt{\frac{1}{2}} & \sqrt{\frac{1}{2}} \end{pmatrix}
\]  

(32)

According to Hamilton Cayley theorem, \( p(\lambda) \) is the characteristic polynomial of the matrix, then

\[
p(A) = A^n + a_{n-1} A^{n-1} + \cdots + a_0 = 0
\]  

(33)

Or

\[
p(A) = (A - \lambda_1 E)(A - \lambda_{n-1} E) \cdots (A - \lambda_n E) = 0
\]  

(34)

\( \lambda_1, \lambda_2, \ldots, \lambda_n \) are the \( n \) eigenvalues of matrix \( A \) (they are not necessarily equal), then

\[
\exp At = \sum_{i=0}^{n} r_{i+1}(t) P_i
\]  

(35)

and

\[
P_0 = E, P_i = (A - \lambda_i E)(A - \lambda_{i+1} E) \cdots (A - \lambda_n E) (i = 1, 2, \ldots, n)
\]

\( r_i(t)(i = 1, 2, \ldots, n) \) is a system of equations

\[
\begin{align*}
\varphi'_1(t) &= \lambda_1 \varphi_1(t) \\
\varphi'_{i+1}(t) &= \varphi_i(t) - \lambda_{i+1} \varphi_{i+1}(t) & (i = 1, 2, \ldots, n-2) \\
\varphi'_n(t) &= \varphi_{n-1}(t) + \lambda_n \varphi_n(t)
\end{align*}
\]  

(36)

Solution satisfying initial condition

\[
\varphi_1(0) = 1, \quad \varphi_2(0) = 0, \quad \cdots, \quad \varphi_n(0) = 0
\]  

(37)
Consider wave function of \( sp^2 \) equivalent hybridization

\[
\begin{align*}
\psi_1 &= \sqrt{\frac{1}{2}} \psi_s + \sqrt{\frac{1}{2}} \psi_{px} \\
\psi_2 &= \sqrt{\frac{1}{6}} \psi_s - \sqrt{\frac{1}{3}} \psi_{py} \\
\psi_3 &= \sqrt{\frac{1}{6}} \psi_s - \sqrt{\frac{1}{3}} \psi_{px} + \sqrt{\frac{1}{2}} \psi_{py}
\end{align*}
\]

Then, matrix formation

\[
\begin{pmatrix}
\psi_1 \\
\psi_2 \\
\psi_3
\end{pmatrix} = \begin{pmatrix}
\sqrt{\frac{1}{2}} & \sqrt{\frac{1}{2}} & 0 \\
\sqrt{\frac{1}{3}} & -\sqrt{\frac{1}{6}} & \sqrt{\frac{1}{2}} \\
\sqrt{\frac{1}{3}} & -\sqrt{\frac{1}{6}} & -\sqrt{\frac{1}{2}}
\end{pmatrix} \begin{pmatrix}
\psi_s \\
\psi_{px} \\
\psi_{py}
\end{pmatrix}
\]

If the wave function obtained is a first-order response function with time, we have

\[
\frac{d}{dt} \begin{pmatrix}
\psi_1(t) \\
\psi_2(t) \\
\psi_3(t)
\end{pmatrix} = \begin{pmatrix}
\sqrt{\frac{1}{2}} & \sqrt{\frac{1}{2}} & 0 \\
\sqrt{\frac{1}{3}} & -\sqrt{\frac{1}{6}} & \sqrt{\frac{1}{2}} \\
\sqrt{\frac{1}{3}} & -\sqrt{\frac{1}{6}} & -\sqrt{\frac{1}{2}}
\end{pmatrix} \begin{pmatrix}
\psi_s(t) \\
\psi_{px}(t) \\
\psi_{py}(t)
\end{pmatrix}
\]

After that, solve the initial value

\[
\begin{align*}
\dot{r}_1(t) &= r_1(t) \\
\dot{r}_2(t) &= r_2(t) - (0.769 + 0.639 i) r_2(t) \\
\dot{r}_3(t) &= r_3(t) - (0.769 - 0.639 i) r_3(t) \\
r_1(0) &= 0, r_2(0) = r_3(0) = 0
\end{align*}
\]

First solve the initial value

\[
\begin{align*}
\dot{r}_1(t) &= e^t \\
r_1(0) &= 1
\end{align*}
\]

The solution is as follows

\[
\begin{align*}
r_1(t) &= e^t \\
\dot{r}_1(t) &= r_1(t)
\end{align*}
\]

Solve the initial value again

\[
\begin{align*}
\dot{r}_2(t) &\approx e^t - (0.769 + 0.639 i) r_2(t) \\
r_2(0) &= 0
\end{align*}
\]

The solution is as follows:

\[
\begin{align*}
r_2(t) &= (0.500 - 0.181 i) e^t - (0.500 - 0.181 i) e^{-0.769 - 0.639 i t}
\end{align*}
\]

3. Results and Discussion

3.1. Geometric Structure of \( \text{Cd}_{43}\text{Te}_{28} \) Microporous Material

We established the geometric structure of the \( \text{Cd}_{n}\text{Te}_{m} \) nanocluster for the initial structure. Thereafter, the nanocluster was optimized by adjusting the supercell size to obtain the \( \text{Cd}_{43}\text{Te}_{28} \) micropore structure. The structures of \( \text{Cd}_{43}\text{Te}_{28} \) are illustrated in Figure 2. The optimized results of the lattice parameters and atomic positions of microporous \( \text{Cd}_{43}\text{Te}_{28} \) are listed in Table 1. The lattice parameters share the same \( a, b \), and \( c \) (16.118 Å) values for \( \text{Cd}_{43}\text{Te}_{28} \), and the atomic positions are all 90.00° in \( \alpha, \beta \), and \( \gamma \). Molecular dynamics simulation shows that \( \text{Cd}_{43}\text{Te}_{28} \) is stable. The results are shown in the supplemental material of Table S1 and Figure S1, S2, Supporting Information. In addition, the optimized atomic coordinates are listed in Table 3, which shows the physical and chemical properties of microporous \( \text{Cd}_{43}\text{Te}_{28} \) for subsequent research. The average diameter for the micropores of \( \text{Cd}_{43}\text{Te}_{28} \) is 8.289 Å (≈0.83 nm), respectively. A microporous material is a material containing pores with diameters less than 2 nm. For example, ETS-10 is a synthetic titanosilicate with a 3D 12-ring channel system with 0.49 × 0.76 nm micropores.[130]

3.2. Band Structure of \( \text{Cd}_{43}\text{Te}_{28} \) Microporous Material

The energy band values of \( \text{Cd}_{43}\text{Te}_{28} \) microporous materials calculated by PBE and LDA potentials are 0.835 and 0.799 eV, respectively. The calculated energy band value may be between 0.799 and 0.835 eV. The delocalization is weak when the energy distribution is smooth, and the density is high. The bandgap width is narrow in these structures, and there is no intersection point between the valence and conduction bands. The 5p orbital of Te has four electrons, and the p energy level can accommodate six electrons, in theory. The 5s orbital of the Cd has two electrons, and the s orbital is filled. Overall, the \( \text{Cd}_{n}\text{Te}_{m} \) microporous structure semiconductor has empty orbitals and is mainly hole conductive. This phenomenon occurs because the Fermi level is closer to the highest point of the valence band. Hence, \( \text{Cd}_{n}\text{Te}_{m} \)
Table 3. Atomic position coordinates obtained after optimization of Cd₄₃Te₂₈ microporous material.

| Cd₄₃Te₂₈   | X       | Y       | Z       |
|------------|---------|---------|---------|
| Cd1        | 15.8430 | 10.0174 | 10.0174 |
| Cd2        | 10.0174 | 15.8430 | 10.0174 |
| Cd3        | 10.0174 | 10.0174 | 15.8430 |
| Cd4        | 7.9649  | 11.4311 | 11.4311 |
| Cd5        | 5.1224  | 14.0294 | 10.9959 |
| Cd6        | 5.1224  | 10.9959 | 14.0294 |
| Cd7        | 2.0889  | 10.9959 | 10.9959 |
| Cd8        | 14.0294 | 5.1224  | 10.9959 |
| Cd9        | 11.4311 | 7.9649  | 11.4311 |
| Cd10       | 10.9959 | 5.1224  | 14.0294 |
| Cd11       | 8.0592  | 8.0592  | 14.6006 |
| Cd12       | 8.1334  | 4.6872  | 11.4311 |
| Cd13       | 4.6872  | 8.1334  | 11.4311 |
| Cd14       | 6.1009  | 6.1009  | 15.8430 |
| Cd15       | 0.2753  | 6.1009  | 10.0174 |
| Cd16       | 10.9959 | 2.0889  | 10.9959 |
| Cd17       | 6.1009  | 0.2753  | 10.9959 |
| Cd18       | 14.0294 | 10.9959 | 10.9959 |
| Cd19       | 10.9959 | 14.0294 | 10.9959 |
| Cd20       | 11.4311 | 11.4311 | 10.9959 |
| Cd21       | 8.0592  | 14.6006 | 10.9959 |
| Cd22       | 8.1334  | 11.4311 | 11.4311 |
| Cd23       | 6.1009  | 15.8430 | 10.9959 |
| Cd24       | 4.6872  | 11.4311 | 11.4311 |
| Cd25       | 0.2753  | 10.0174 | 11.4311 |
| Cd26       | 14.6006 | 8.0592  | 10.9959 |
| Cd27       | 15.8430 | 6.1009  | 10.9959 |
| Cd28       | 11.4311 | 8.1334  | 11.4311 |
| Cd29       | 11.4311 | 4.6872  | 11.4311 |
| Cd30       | 8.0592  | 8.0592  | 11.4311 |
| Cd31       | 7.9649  | 4.6872  | 11.4311 |

Table 3. Continued.

| Cd₄₃Te₂₈   | X       | Y       | Z       |
|------------|---------|---------|---------|
| Cd32       | 4.6872  | 7.9649  | 4.6872  |
| Cd33       | 4.6872  | 4.6872  | 7.9649  |
| Cd34       | 1.5177  | 8.0592  | 8.0592  |
| Cd35       | 2.0889  | 5.1224  | 5.1224  |
| Cd36       | 10.0174 | 0.2753  | 6.1009  |
| Cd37       | 8.0592  | 1.5177  | 8.0592  |
| Cd38       | 5.1224  | 2.0889  | 5.1224  |
| Cd39       | 10.9959 | 10.9959 | 2.0889  |
| Cd40       | 6.1009  | 10.0174 | 0.2753  |
| Cd41       | 10.0174 | 6.1009  | 0.2753  |
| Cd42       | 8.0592  | 8.0592  | 1.5177  |
| Cd43       | 5.1224  | 5.1224  | 2.0889  |
| Te1        | 12.9744 | 9.7538  | 9.7538  |
| Te2        | 9.7538  | 12.9744 | 9.7538  |
| Te3        | 9.7538  | 9.7538  | 12.9744 |
| Te4        | 6.5871  | 13.1914 | 13.1914 |
| Te5        | 6.3920  | 9.7263  | 9.7263  |
| Te6        | 2.9269  | 13.1914 | 9.5312  |
| Te7        | 2.9269  | 9.5312  | 13.1914 |
| Te8        | 13.1914 | 6.5871  | 13.1914 |
| Te9        | 13.1914 | 2.9269  | 9.5312  |
| Te10       | 9.7263  | 6.3920  | 9.7263  |
| Te11       | 9.5312  | 2.9269  | 13.1914 |
| Te12       | 6.3645  | 6.3645  | 12.9744 |
| Te13       | 6.3645  | 3.1439  | 9.7538  |
| Te14       | 3.1439  | 6.3645  | 9.7538  |
| Te15       | 13.1914 | 13.1914 | 6.3920  |
| Te16       | 13.1914 | 9.5312  | 2.9269  |
| Te17       | 9.5312  | 13.1914 | 2.9269  |
| Te18       | 9.7263  | 9.7263  | 6.3920  |
| Te19       | 6.3645  | 12.9744 | 6.3645  |
| Te20       | 6.3645  | 9.7538  | 3.1439  |
can be considered a p-type semiconductor. Semiconductors with this type of microporous structure may exhibit an excellent catalytic performance. For example, Li et al. found microporous organic polymers (MOPs) as heterogeneous photocatalysts for visible light promotion.

3.3. Density of States of Cd$_{43}$Te$_{28}$ Microporous Material

In Figure 3, the density of states (DOS) diagrams of Cd$_{43}$Te$_{28}$ are given. The main peaks of the electron density distribution occur at −1.52 eV for Cd$_{43}$Te$_{28}$. The structure is relatively stable because of the main peaks located in the direction of negative energy. Moreover, the zero field can be observed near the Fermi level, and the Cd$_{43}$Te$_{28}$ status as a semiconductor has been confirmed from the energy band diagram. The energy region of the three structures fluctuates significantly and is typical of a p-type band structure. The p electrons are relatively localized, which corresponds with the narrow bandgap. The partial density of states (PDOS) was analyzed for Cd$_{43}$Te$_{28}$. Figure 3 illustrates that the change in the Cd$_{43}$Te$_{28}$ structure DOS curve is the largest, and Cd contributes substantially to the Cd$_{43}$Te$_{28}$ structure. The contribution of Cd was confirmed by the presence of obvious peaks throughout the energy range.

3.4. Deformation Charge Density and Bonding of Cd$_{43}$Te$_{28}$ Microporous Material

The deformation charge density is calculated by DFT and can be obtained via contribution from four bonding and electronic features. The deformation charge densities of Cd$_{43}$Te$_{28}$ are shown in Figure 4. The deformation charge density scale indicates the charge value. The red and blue are represented as the increase and decrease of the electron distribution respectively. The electrons in the positive region are convergent, while they are divergent in the negative region. The red and white regions represent numerous electrons gathering, and the deformation charge density is positive. The established BBC model was used to convert the value of Hamiltonian into the value of energy.

| Cd$_{43}$Te$_{28}$ | X     | Y     | Z    |
|-------------------|-------|-------|------|
| Te21              | 3.1439| 9.7538| 6.3645|
| Te22              | 12.9744| 6.3645| 6.3645|
| Te23              | 9.7538| 6.3645| 3.1439|
| Te24              | 9.7538| 3.1439| 6.3645|
| Te25              | 6.3920| 6.3920| 6.3920|
| Te26              | 6.5871| 2.9269| 2.9269|
| Te27              | 2.9269| 6.5871| 2.9269|
| Te28              | 2.9269| 2.9269| 6.5871|

Figure 3. a,c) Band structure and b,d) partial DOS of Cd$_{43}$Te$_{28}$ microporous material.
bonding (Table 4). Using Equation (11), the deformation bond energy is \(-0.0797\) eV for Cd\(_{43}\)Te\(_{28}\). We developed a method to accurately analyze the chemical bonding and electronic properties of microporous semiconductor materials. In conclusion, our calculations provide a theoretical reference for the bonding properties of Cd\(_n\)Te\(_m\) microporous semiconductor materials.

3.5. Geometric Topological Bonding and Wave Function

By introducing the phase into the chemical bond, the topological bonding information is obtained.

Take \(z\) as the vertical direction

\[
\begin{align*}
\vec{f}(x_i) &= x_i + (r_x e^{X_i} + A \sin [\nu] \cdot \cos [\mu]) \\
\vec{f}(y_i) &= y_i + (r_y e^{X_i} + A \sin [\nu] \cdot \sin [\mu]) \\
\vec{f}(z_i) &= z_i + \cos [\nu]
\end{align*}
\]

Take \(y\) as the vertical direction

\[
\begin{align*}
\vec{f}(x_i) &= x_i + (r_x e^{X_i} + A \sin [\nu] \cdot \cos [\mu]) \\
\vec{f}(y_i) &= y_i + B \cos [\nu] \\
\vec{f}(z_i) &= z_i + (r_y e^{X_i} + A \sin [\nu] \cdot \sin [\mu])
\end{align*}
\]

Table 4. The deformation charge density \(\delta\rho(\vec{r})\) and deformation charge of bond energy \(\Delta V_{bc}(\vec{r})\), as obtained using BBC model. \((\varepsilon_0 = 8.85 \times 10^{-12} \text{C}^2 \text{N}^{-1} \text{m}^{-2}, \varepsilon = 1.60 \times 10^{-19} \text{C}, r_j = 1.44 \text{Å} \text{(Cd)}, r_{ij} = 1.38 \text{Å} \text{(Te)}, |\vec{r}_i| = |\vec{r}_j| = d_{ij}/2 = 1.49 \text{Å})\).

| Structure  | \(\delta\rho\)hole–electron (\(\vec{r}_i\)) [e Å\(^{-3}\)] | \(\delta\rho\)binding–electron (\(\vec{r}_i\)) [e Å\(^{-3}\)] | \(\Delta V_{bc}^{\text{binding}}(\vec{r}_i)\) [eV] |
|------------|-----------------|-----------------|-----------------|
| Cd43Te28   | 0.0389          | 0.0541          | 0.0797          |

Figure 4. Deformation charge density of Cd\(_{43}\)Te\(_{28}\) microporous material.

Figure 5. The geometric topological bonding a) \(A = 8 = 1, \chi = 0, u = 6, \nu = 6\), b) \(A = 0.5, B = 1, \chi = 0, u = 6, \nu = 6\), and c) \(A = 1, B = 0.5, \chi = 0, u = 6, \nu = 6\) of Cd\(_{43}\)Te\(_{28}\) microporous material using BBC model.
Cd43Te28 microporous material.

The operation of the magic cube matrix wave function. Fm(n), dynamic.\(^{(38)}\) which is related to the experimental chemical reaction Equation (49)

Letter by itself (e.g., F) means turn that face 90° clockwise with direction. The subscript m represents the number of revolutions. A letter in the context of magic cube matrix. F

In Section 2.3, we discuss the time-dependent first-order response wave function. For topological chemical bonds, we need to use topological wave function. We call magic cube (Rubik’s cube)\(^{(39)}\) wave function, as shown in Figure 5. The calculated parameters are shown in Table 5. Equation (49)–(51) can obtain the topological form of atoms, which is related to the experimental chemical reaction dynamic.\(^{(38)}\)

In Table 5. The atomic position coordinates and the atomic radius \(r\) of Cd43Te28 microporous material.

| Element   | \(X\)  | \(Y\)  | \(Z\)  | \(r\) |
|-----------|--------|--------|--------|-------|
| Cd-24     | 4.6872 | 11.4311| 8.1534 | 1.44  |
| Te-6      | 2.9269 | 13.1914| 9.5312 | 1.38  |

Take \(x\) as the vertical direction

\[
\begin{align*}
  f(x_i) &= x_i + B\cos[\psi] \\
  f(y_i) &= y_i + (r, e^{-x^2}) + \sin[\psi] \cdot \sin[u] \\
  f(z_i) &= z_i + (r, e^{-x^2}) + \sin[\psi] \cdot \cos[u]
\end{align*}
\] (51)

\(x, y,\) and \(z\) represent the position coordinates of the atom, \(r\) represents the radius of the atom, \(\psi\) is electron shielding parameter, \(A\) and \(B\) represent the amplitude of the wave, and \(u\) and \(v\) represent the phase of the wave. We use Equation (49)–(51) to calculate the geometric topological bonding of Cd43Te28 microscopic semiconductor materials, as is shown in Figure 5. The calculated parameters are shown in Table 5. Equation (49)–(51) can obtain the topological form of atoms, which is related to the experimental chemical reaction dynamic.\(^{(38)}\)

\[
\begin{align*}
  f(x_i) &= x_i + B\cos[\psi] \\
  f(y_i) &= y_i + (r, e^{-x^2}) + \sin[\psi] \cdot \sin[u] \\
  f(z_i) &= z_i + (r, e^{-x^2}) + \sin[\psi] \cdot \cos[u]
\end{align*}
\] (51)

Equation (51) gives the matrix transformation process of the magic cube wave function operated by the rotation operator.

Equation (52) gives the matrix transformation process of the magic cube wave function operated by the rotation operator.

In this study, the band structure, DOS, and deformation charge density of Cd43Te28 microporous materials were determined using DFT calculations. The bandgap value of Cd43Te28 structures is 0.835 eV. For semiconductor microporous materials, it is necessary to regulate the physical and chemical properties of a novel structure from the perspective of semiconductor applications. In addition, the established BBC model was used to convert the value of Hamiltonian into the bonding value. We provide a method for describing topological chemical bonds by atomic coordinates and wave phases. We also discuss the dynamic process of the wave function with time and the magic cube matrix. This work provides an innovative method and technology for the
accurate analysis of the bond and electronic properties for microporous semiconductor materials.

Supporting Information
Supporting Information is available from the Wiley Online Library or from the author.

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Conflict of Interest
The authors declare no conflict of interest.

Data Availability Statement
The data that support the findings of this study are available from the corresponding author upon reasonable request.

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CdTe semiconductors, density functional theory calculations, microporous materials, topological bonding, wave functions

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