Systematic strain-induced bandgap tuning in binary III–V semiconductors from density functional theory

Badal Mondal and Ralf Tonner-Zech
1 Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Universität Leipzig, 04103 Leipzig, Germany
2 Fachbereich Physik, Philippus-Universität Marburg, 35032 Marburg, Germany
E-mail: ralf.tonner@uni-leipzig.de

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Abstract
The modification of the nature and size of bandgaps for III-V semiconductors is of strong interest for optoelectronic applications. Strain can be used to systematically tune the bandgap over a wide range of values and induce indirect-to-direct transition (IDT), direct-to-indirect transition (DIT), and other changes in bandgap nature. Here, we establish a predictive first-principles approach, based on density functional theory, to analyze the effect of uniaxial, biaxial, and isotropic strain on the bandgap. We show that systematic variation is possible. For GaAs, DITs are observed at 1.56% isotropic compressive strain and 3.52% biaxial tensile strain, while for GaP an IDT is found at 2.63% isotropic tensile strain. We additionally propose a strategy for the realization of direct-to-indirect transition by combining biaxial strain with uniaxial strain. Further transition points are identified for strained GaSb, InP, InAs, and InSb and compared to the elemental semiconductor silicon. Our analyses thus provide a systematic and predictive approach to strain-induced bandgap tuning in binary III–V semiconductors.

1. Introduction
Semiconductor compounds attract a great amount of attention, both in science and technology, due to their immense application range in areas such as optoelectronics and integrated circuits [1, 2]. One of the major goals in basic and applied research is to tailor the optical properties of semiconductor materials to a target application. The most important fundamental property determining these properties is the material’s bandgap. For example, materials for optical telecommunication applications require direct bandgaps in the range of 0.80–0.95 eV [3–5], while a range of 0.5–2.0 eV is necessary for materials used in efficient solar cells [6–9]. One material class that is especially versatile in this respect are compound semiconductors, specifically the III-V semiconductors composed of elements from group 13 and 15 of the periodic table of elements [2, 5, 10–22]. In the last decades, the optical properties of this material class have been intensively investigated [2, 10–14, 22–36] and several strategies have emerged to fine-tune the bandgap. Changing the nature of the chemical elements and their relative composition is a powerful approach to vary the gap over a wide range of energies [37–44]. However, changing the chemical composition is not always possible. One reason for this lies in the constraints in the growth characteristics of precursor molecules for the chemical vapor deposition techniques often used to grow these materials. Another reason is the thermodynamic instabilities of some elemental compositions [3, 14, 37, 44–48].

An alternative and sometimes also complementary approach to vary the bandgap is strain engineering. This can be achieved through external effects such as: applying pressure on the system [23, 24, 27–36], altering the temperature of the system, or changing the substrate in epitaxial growth processes [13, 16, 19, 37–42, 45, 46, 49–62]. All of these approaches result in structural strain in the system because of the deviation of one or several lattice parameters of the material from their equilibrium values. The effects on the electronic structure from
investigation of strain effects has recently found renewed interest in the applied parameters are kept wide range of applications semiconductors: GaAs and GaP. These materials are not only interesting for basic research but also support a Furthermore, no systematic theoretical study is yet available that predicts optical properties of strained materials. This approach can also successfully be used for predicting properties when applying a wide range of strains to the lattice parameter of an empirical methods such as the local/nonlocal empirical pseudopotential method [63–71], the semi-empirical tight-binding method [72–84], the k·p method [85–90]; or by (b) first-principles methods [91–98] such as density functional theory (DFT) [91, 99–104]. Although empirical and semi-empirical methods are computationally efficient and often easy to apply, they rely on many empirical fitting parameters. This strongly lowers their ability to predict properties for new materials, which is a core goal in computational materials design [105]. In contrast, first-principles methods allow the calculation of the electronic structure without the need for empirical fitting parameters.

One of the most widely used first-principles approaches in material science is DFT. The crucial ingredient here is the density functional. Functionals following the generalized gradient approximation (GGA) often lead to an excellent agreement of computed lattice parameters with experimental data. However, they are known to show very large errors for bandgaps [105–109]. Hybrid functionals such as HSE06 [110] and GW-based methods [95–98] can solve this issue but are computationally expensive. Previously, we and others successfully used the exchange-correlation functional, developed by Tran and Blaha, to predict the electronic properties of unstrained III–V compound semiconductors without empirical adjustments or application of scissor operators [105, 111–117]. Although this functional contains one global system-dependent parameter, this parameter is derived from the density and two fitted parameters only without adjustment to experimental values. Here, we will show that this approach can also successfully be used for predicting properties when applying a wide range of strains to these materials.

Although strain engineering is an established field for III–V semiconductors [2, 45, 87, 118, 119], the investigation of strain effects has recently found renewed interest in the field of nanowires [120–128]. Furthermore, no systematic theoretical study is yet available that predicts optical properties of strained materials of this kind without empirical adjustments. We now set out to reliably predict the optical properties of strained materials over a wide range of strains. This will ultimately enable computational materials design approaches in strain engineering of established and upcoming materials.

This work will establish the methodology and highlight the challenges of predictive modelling. Thus, we focus our analysis of strain effects on the electronic structure of the most widely investigated binary III–V semiconductors: GaAs and GaP. These materials are not only interesting for basic research but also support a wide range of applications (either as binary materials or as a host material for multinary compounds) in microelectronics, solar cells, laser technology, and LEDs [2–9, 14–21]. To show the general applicability of our approach, selected data on the materials Si, GaSb, InP, InAs, and InSb are included.

In this work, we present and validate a computational approach predicting the size and nature of the bandgap of III–V semiconductor materials over a wide range of strain values. The ultimate goal is to provide guidelines for future experimental work on strained materials.

2. Model

In this study we model uniaxial, biaxial, and isotropic strain. Figure 1 schematically shows which lattice parameters are kept fixed and which are relaxed in the modelling of these three types of strain. The materials investigated are all feature zincblende structures. The growth direction in the ‘theoretical epitaxy’ approach applied (see below) is taken to be [001] in this study and is defined as the z-direction in our modelling approach. We limit our analysis of uniaxial strain to the application of strain along the growth direction only. This uniaxial (compressive) strain is experimentally realized most often by applying pressure. Here, we model this by varying the lattice parameter in the z-direction while relaxing the in-plane lattice parameters (figure 1(a)). In the spirit of a systematic study, we also study uniaxial tensile strain over the same range of values. However, the experimental realization of expanding lattice parameters is typically limited to small strain values (e.g. by increasing the temperature or applying shear stress). The major approach to produce biaxially strained materials is epitaxial growth on a substrate with a different lattice parameter \((a_s)\). We thus fix the in-plane lattice parameters \((a_x, a_y)\) to the lattice parameter of an (imaginary) substrate \((a_s)\) while varying the parameter in the growth direction (figure 1(b)). In this case, we consider the structural strain imposed by a substrate but neglect the electronic influence for the modelling (theoretical epitaxy) [45, 119]. Isotropic strain is then consequently modelled by not constraining any lattice parameter and increasing (decreasing) all lattice parameters by the same amount (figure 1(c)).
3. Computational details

Computations were carried out with DFT-based approaches as implemented in the Vienna Ab initio Simulation Package (VASP 5.4.4) [101, 130–133], using plane-wave basis sets in conjunction with the projector augmented wave (PAW) method [134, 135]. The primitive zincblende cell was used throughout. The basis set energy cutoff of 450 eV, the electronic energy convergence criteria of $10^{-6}$ eV, and the force convergence of $10^{-2}$ eV/Å were used. Reciprocal space was sampled with a $10 \times 10 \times 10$ Γ-centered Monkhorst-Pack k-point mesh [136]. We used these settings for all the solids studied in this work. The convergence test for k-mesh and plane wave cutoff are presented in figure S1. Optimizations of the primitive cells were performed using the Perdew–Burke–Ernzerhof (PBE) exchange-correlation functional [106] with the semi-empirical dispersion correction scheme DFT-D3 with a Becke-Johnson type damping function [137, 138]. We also tested other approaches to describe dispersion interactions (table S1, figure S2). The best agreement between the optimized and experimental lattice parameters were found using PBE-D3(BJ) approach. Other methods to treat dispersion interaction delivered less good agreement. The geometry optimizations were carried out by the consecutive volume and position optimization until convergence was reached. For every set of lattice parameter values investigated, all atomic positions were optimized.

For the bandgap and band structure calculations, the TB09 functional was used [111] including spin–orbit coupling. This had previously been used to give an excellent agreement with the experimental bandgaps for this compound class [105, 111–116]. The band energies for all the different configurations were re-normalized to the respective VBM. We limited our calculations to a range of ±10% strain by applying constrained optimizations as outlined in the previous section. This is in the order of magnitude of pressures (10 to several 100 GPa) achievable in modern experiments [33, 139–150]. We indicate tensile strain with a '+' sign to emphasize the positive strain value and to make it easier for the reader to distinguish it from compressive strain values, which are denoted with a '-' sign.

The contribution of the atomic orbitals at the different k-points on the bands was calculated by projecting the plane waves on the minimal basis set using LOBSTER [151, 152].

4. Results

4.1. Unstrained structures

Before we discuss the influence of strain, the unstrained materials investigated here shall briefly be presented. Regarding the sign convention, we define positive strain to correspond to expansion (tensile strain) and negative strain as compression (compressive strain). The strain values were calculated according to equation (1).

\[
\text{strain(\%)} = \frac{a_f - a_{\text{eqm}}}{a_{\text{eqm}}} \times 100
\]  

Here, $a_f$ is the lattice parameter in the strained structure while $a_{\text{eqm}}$ is the equilibrium lattice parameter. The equilibrium lattice parameters for all materials investigated were computed with the PBE-D3(BJ) approach and are given in table 1. The good agreement with the experimental lattice parameters (maximum deviation of 0.09 Å or 1.3%) lends confidence to the accuracy of the theoretical approach.
4.2. Gallium arsenide

4.2.1. Isotropic strain

First, we present the bandgap variation of GaAs under the application of isotropic strain in a range of ±10% around the unstrained lattice parameter. Figure 2 shows the variation of the energy difference between the conduction band \( (\text{CB}) \) and the valence band \( (\text{VB}) \) at the \( \Gamma \) point \( (\Delta E_\Gamma) \), as well as the bandgap \( (E_g) \), as a function of strain. Here, and throughout the manuscript, we distinguish between these two energy differences. For a direct bandgap material, both values are the same. If \( E_g \) is smaller than \( \Delta E_\Gamma \) this indicates an indirect bandgap. A strain value where the two curves start deviating thus indicates a direct-to-indirect (DIT) bandgap transition point.

Under tensile strain, \( E_g \) decreases until, at \(+6.78\%\) strain, the bandgap vanishes, corresponding to a semiconductor-to-metal transition (SMT). In this case, the \( E_g \) curve coincides with the \( \Delta E_\Gamma \) curve throughout, indicating a direct bandgap. Under compressive strain, however, the \( E_g \) curve initially follows the \( \Delta E_\Gamma \) curve until \( -1.56\% \) strain, where the \( E_g \) curve then separates from the \( \Delta E_\Gamma \) curve. Although \( \Delta E_\Gamma \) still increases under further strain, the bandgap starts to decrease. Thus, we have a DIT point here.

To understand the origin of this deviation, we look at the band structures computed at each strain value. The band structures can be found in the supporting information (figures S3 (a), (b)). We find that the VBM remains at the \( \Gamma \) point not only here but for all materials and strain regimes investigated. Only the CBM changes its position in k-space when strain is applied. Thus, the change in CBM under compressive strain determines the change in the nature of bandgap. Figure 3 shows the change in CB energies for strained GaAs relative to their values for the unstrained structure at four high-symmetry points in reciprocal space: \( \Gamma \), \( L \), \( \Delta_m \), and \( X \) points.

This shows that the CB energies at the \( \Gamma \) and \( L \) points decrease under tensile strain with a slight increase for \( \Delta_m \) and \( X \) points. The largest change is found at the \( \Gamma \) point, followed by \( L \), \( \Delta_m \), and \( X \). As unstrained GaAs is a direct bandgap semiconductor, this signifies that the bandgap remains direct under tensile strain, to begin with. Subsequently, at \(+6.78\%\) strain, the CBM and VBM become degenerate, which results in the SMT.

For compressive strain, however, the CB energies at the \( \Gamma \) and \( L \) point increase while a slight decrease is found at the \( \Delta_m \) and \( X \) points (figure 3). This results in an increase in the direct bandgap for small strain values. Since CB at the \( \Gamma \) point changes the most with strain, beyond \(-1.56\%\) strain it supersedes the energy at the \( L \) point. This results in the CBM shifting from the \( \Gamma \) to the \( L \) point and a DIT. CB energy at the \( \Gamma \) point increases

Table 1. Computed (PBE-D3(BJ)) optimized unstrained lattice parameters (Å) for the materials investigated in comparison to experimental reference values at 0 K.

| System  | Si   | GaP   | GaAs  | GaSb  | InP   | InAs  | InSb  |
|---------|------|-------|-------|-------|-------|-------|-------|
| Calculation | 5.421 | 5.474 | 5.689 | 6.134 | 5.939 | 6.138 | 6.556 |
| Experiment \([38, 129]\) | 5.430 | 5.442 | 5.642 | 6.082 | 5.861 | 6.050 | 6.469 |

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For compressive strain, however, the CB energies at the \( \Gamma \) and \( L \) point increase while a slight decrease is found at the \( \Delta_m \) and \( X \) points (figure 3). This results in an increase in the direct bandgap for small strain values. Since CB at the \( \Gamma \) point changes the most with strain, beyond \(-1.56\%\) strain it supersedes the energy at the \( L \) point. This results in the CBM shifting from the \( \Gamma \) to the \( L \) point and a DIT. CB energy at the \( \Gamma \) point increases
further resulting in a steep increase of $\Delta E_{\Gamma}$ for high strain values (figure 2). CB at the L point increases much slower in energy, flattening the $E_g$ curve and even producing bandgap decrease at high compressive strain (figure 2).

Further, by comparing the difference in CB energies at the $\Gamma$ point and other k-points $P (\Delta E_{CB} = E_{CB,P} - E_{CB,\Gamma};$ with $P = \Gamma, L, \Delta_m,$ and $X$) for isotropically strained GaAs. Colored areas indicate at which k-point we find the CBM for the given value of compressive strain. The color scheme: $\Gamma$ (red), L (blue), $\Delta_m$ (purple), and X (olive).

## 4.2.2. Biaxial strain

The effect of the biaxial strain on the bandgap is shown in figure 5 (band structures are shown in figures S3(d), (e)). The bandgap decreases under both compressive and tensile strain. During compression, the $E_g$ curve coincides with $\Delta E_{\Gamma}$ throughout. The CBM always remains at the $\Gamma$ point, and hence, the bandgap remains direct. Only for very high compressive strain values (beyond $\sim 7.86\%$), the CBM and VBM become degenerate,
leading to an SMT. For tensile strain, a DIT is found at $+3.52\%$ strain, exemplified by the $E_{\text{g}}$ curve splitting from $\Delta E_{\Gamma}$ in figure 5.

Under further tensile strain, the bandgap continues to decrease until GaAs become a semimetal at $+8.00\%$ strain. Thus, we observe a semiconductor to semimetal transition (SsMT). By comparing the difference in CB energies at the $\Gamma$, L, $\Delta_m$, and X points (figure S4) we find the DIT to correspond to a $\Gamma$ to $\Delta_m$ transition. No further transition points are found here.

4.2.3. Uniaxial strain
The uniaxial strain model in our case is equivalent to the biaxial strain model. This is true because we consider the [001] crystal orientation in the zincblende crystal grown on the [001] surface of another zincblende substrate, and the uniaxial strain is then applied in the $\langle 100 \rangle$ direction (figure 1(a)). In this configuration, relaxing the lattice parameter in the $z$-direction at fixed in-plane ($x$ and $y$) lattice parameters ($a$) is equivalent to fixing it in the $z$-direction at the value $a$, and relaxing the in-plane parameters. For the uniaxial strain in other crystal orientations or directions, this equivalence is not true, because of finite off-diagonal stress tensor elements [118, 153, 154].

Therefore, we use the data from the previous subsection and now present them as a function of the out-of-plane lattice parameter (figure 6). This is essentially a mirrored version of figure 5 with a changed scaling of the x-axis. Now, we find the DIT at $-7.30\%$ strain, the SsMT at $-15.43\%$ strain, and the SMT at $+17.73\%$ strain, respectively.

4.2.4. Combining biaxial and uniaxial strain
Uniaxial and biaxial strain are shown in the previous sections to be useful strategies to tune the magnitude of the bandgap. However, one major goal in tuning the electronic structure is changing the nature of the bandgap. As shown in the previous subsection, this however, can not be achieved via biaxial compressive strain, which is one of the most common experimental realizations of strain via epitaxial growth. We will now show that in a new strategy by combining this biaxial compressive strain with uniaxial strain changes in the nature of the bandgap can in fact be achieved.

In a thought experiment (figures 7, S5), the desired material (GaAs) is first ‘grown’ epitaxially on a substrate with a smaller lattice constant (e.g., GaP), resulting in compressive biaxial strain (here: $-3.78\%$). Such epitaxial growth would lead to expansion of the $z$-lattice parameter. Subsequently, uniaxial compressive strain (e.g., pressure) could be applied along the $z$-direction to compress the $z$-lattice parameter. We assume that the in-plane lattice parameters would not relax upon compression of the $z$-lattice parameter. We thus model a case here where strain is accumulated inside the epitaxial layer without creating defects. In this case, we find a DIT point at $-3.2\%$ uniaxial strain (figure 8).

Next, we further generalize this strategy. Figure 9 shows the required uniaxial compressive strain for the DIT in biaxial compressively strained GaAs. No transition can be achieved for biaxial compressive strain below $1.56\%$, as both the biaxial and isotropic strain would have the same direct nature of the bandgap (figures 7, S6).
A similar strategy can be applied for the indirect to direct transition (IDT) in biaxial tensile strained GaAs (figure S6). In this case, one would need to expand the \( z \)-lattice parameter for the transition. Experimentally, this can be achieved e.g., by thermal expansion. As shown in figure S7, this however, is only reasonable for biaxial strain smaller than 4.5%. For higher biaxial strain the large required amount of uniaxial tensile strain can not be achieved by thermal expansion only.

### 4.3. Gallium phosphide

Gallium phosphide is an indirect bandgap semiconductor. Next, we demonstrate the application of strain on the bandgap engineering. Figure 10 shows the variation in CB energy for GaP under isotropic strain at the \( \Gamma \), \( L \), \( \Delta_m \) and \( X \) points relative to their unstrained values (band structures are shown in figures S3(f), (g)).

For compressive strain, the CB at \( \Gamma \) and \( L \) point increases in energy, while it decreases at the \( \Delta_m \) and \( X \) points. As GaP is an indirect bandgap semiconductor at equilibrium, the nature of the bandgap thus does not change. For tensile strain, the CB energy at the \( \Gamma \) and \( L \) points decreases strongly while we find a small increase at the \( \Delta_m \) and \( X \) points. This lead to a shift of the indirect bandgap from \( \Delta_m \) to \( L \) at +1.43% tensile strain (figure 11).
the slope for the energy at the $\Gamma$ point is largest (figure 10), we find an indirect to direct transition (IDT) at $+2.63\%$ strain (figures 11, S8).

The result for biaxial strain is shown in figure 12 (band structures are shown in figures S3(h), (i)). Here, we find no change in the nature of the bandgap throughout the entire range of compressive and tensile strain. The bandgap remains indirect throughout. For very high strain values, we find SsMTs at $+8.45\%$ and $-9.83\%$ strain.

The uniaxial conversion of the data in figure 12, as is explained for GaAs case, would not have any further special interest (figure S9). Similar to GaAs, by combining biaxial and uniaxial strain in GaP one can in principle achieve IDT. However, this would require large uniaxial tensile strain ($>8\%$), which can not be realized by thermal expansion (figure S10).

### 4.4. Silicon, GaSb, InP, InAs, and InSb

We also applied the approach outlined in detail for GaAs and GaP to other interesting semiconductor materials. Tables 2 and 3 summarizes the main results for Si, GaSb, InP, InAs, and InSb. In all cases, the VBM stays at the $\Gamma$ point throughout the strain regimes applied. Thus, the position of the CBM in reciprocal space determines the nature of the bandgap.
Si and GaP are indirect bandgap semiconductors in their equilibrium structure while the other materials discussed show direct bandgaps. Accordingly, Si and GaP show IDTs while the other materials show DITs. The strain values where these transitions are found, for isotropic and biaxial strain, are shown in columns 3 and 4 of table 2. For the isotropic strain case, the IDTs are found for tensile strain as already discussed for GaP in the previous section. The value for Si is so high (+10.31%) that it will certainly be out of range for any experiment.

The DITs are found for isotropic compressive strain throughout, with strain values ranging from −1.00% (GaSb) to −7.41% (InAs).

For biaxial strain, DITs are found only for GaAs, GaSb, and InP. In all cases, a significant tensile strain would be necessary. For many materials, transitions are found to other k-points in reciprocal space where the nature of the bandgap stays indirect. This is shown in the right-hand part of the table. [more details are shown in figures S11, S12, and S13.]

Notably, In-based compound semiconductors show the DIT points at much higher strain values compared to Ga-based materials. Figure 13 shows the contribution of the atomic orbitals to the CB for unstrained GaAs and InAs. At the decisive points in k-space (Γ, L, and X points) the group III elements show the major orbital contributions to CB. Furthermore, while the s-orbital contributions (Ga(4s), In(5s)) dominate at the Γ point, the L point and the X point show high p-orbital contributions (Ga(4p), In(5p)). Since the energy gap between 5s and 5p orbitals is significant...
5p orbital in In is much higher than 4s and 4p in Ga, changing group III from Ga to In increases the energy difference between \( \Gamma \) and \( \Delta \) and \( L \), respectively (see figure 14). Under strain, the decrease of these energy differences ultimately results in the shift of CBM from the \( \Gamma \) to the \( L \) and/or \( X \) point (figures S3, S14). Therefore, the higher this relative energy difference, the higher the requirement of the amount of strain needed to reach the

**Table 2.** Change in the nature of bandgap for different III-V semiconductor materials for isotropic and biaxial strain.

| System | Transition Path | Isotropic (%) | Biaxial (%) |
|--------|-----------------|--------------|-------------|
| Si     | IDT +10.31\( ^{b} \) | \( \times \)  | \( \times \) |
| GaP    | IDT +2.63       | \( \times \)  | \( \times \) |
| GaAs   | DIT -1.56       | +3.52        | \( \Gamma \rightarrow \Delta \rightarrow X \) |
| GaSb   | DIT -1.00       | +3.71        | \( \Gamma \rightarrow \Delta \rightarrow \Delta \) |
| InP    | DIT -4.40       | +7.66        | \( \Gamma \rightarrow \Delta \rightarrow \Delta \) |
| InAs   | DIT -7.41       | \( \times \)  | \( \Gamma \rightarrow \Delta \rightarrow \Delta \) |
| InSb   | DIT -5.18       | \( \times \)  | \( \Gamma \rightarrow \Delta \rightarrow \Delta \) |

\(^{a}\) Direct to indirect transition (DIT) and indirect to direct transition (IDT).

\(^{b}\) Estimated using linear extrapolation.

\( \times \) No transitions within \( \pm 10\% \) strain.

**Table 3.** Semiconductor to metal transition (SMT) and semiconductor to semimetal transition (SsMT) points for different III-V semiconductor materials under isotropic and biaxial strain. \( \Delta E_{\Gamma} \) corresponds to the energy difference between CB and VB at the \( \Gamma \) point.

| System | \( \Delta E_{\Gamma} \) (eV) | Isotropic (%) | Biaxial (%) | Isotropic (%) | Biaxial (%) |
|--------|-----------------------------|--------------|-------------|--------------|-------------|
| Si     | 3.14                        | +15.00\(^{a}\) | \( \times \)  | \( \times \)  | +3.70, -6.50 |
| GaP    | 2.99                        | +13.00\(^{a}\) | \( \times \)  | \( \times \)  | +8.45, -9.83 |
| GaAs   | 1.81                        | +6.67        | -7.86       | \( \times \)  | +8.00       |
| GaSb   | 0.64                        | +2.85        | -5.00       | \( \times \)  | +5.07       |
| InP    | 1.43                        | +8.20        | -9.90       | \( \times \)  | +10.38      |
| InAs   | 0.36                        | +2.10        | +4.74, -4.36| \( \times \)  | \( \times \) |
| InSb   | 0.03                        | +0.34        | +0.34, -0.34| \( \times \)  | \( \times \) |

\(^{a}\) Estimated using linear extrapolation.

\( \times \) No transitions within \( \pm 10\% \) strain.

Figure 12. Biaxial strain effects on the bandgap of GaP. The energy difference between CB and VB at the \( \Gamma \) point (\( \Delta E_{\Gamma} \), blue), the bandgap (\( E_{g} \), magenta), and the semiconductor to semimetal (SsMT) transitions are shown. The solid orange line indicates \( E_{g} \) for the unstrained structure (2.36 eV).
This results in DIT points at larger strain values for In-based compounds in comparison to the Ga-based compounds. Note that, as the above reasoning is qualitative, for simplicity, we do not consider the $\Delta_m$ point here.

Table 3 summarizes the SMTs and SsMTs for the compound semiconductors investigated. These transitions depend on the closing of the CBM and VBM gaps. As the VBM always remains at the $\Gamma$ point, these transition points therefore depend on $\Delta E_{\Gamma}$. Figure 15 shows the SMTs under isotropic strain for different systems in relation to their corresponding $\Delta E_{\Gamma}$. As the $\Delta E_{\Gamma}$ increases, so does the S(s)MT values.

In table 4, we compare our calculated results with the available experimental findings. The results match quite well. In experiments, the DIT points were measured in terms of applied hydrostatic pressure. Using the third-order Birch-Murnaghan equation [155] we converted the measurement in terms of strains. We used reference [156, 157] for the bulk modulus and and its first derivative data for the conversion. For GaAs, the strain region when CBM is visible at the L point is very small (only 0.72% strain window), figure 4. Therefore, we conclude that in the experiment this region was most likely missed (table 4, 3rd row last column). For InSb a deviation of 0.21 eV was found for the equilibrium bandgap. This, in turn, would result in the overestimation of the DIT point in our calculation (table 4, 7th row last column).

Figure 13. Atom resolved orbital contributions for unstrained GaAs and InAs CB. Solid sky blue: Ga(4s), dotted sky blue: In(5s), solid orange: Ga(4p), dotted orange: In(5p), solid green: As(4s) in GaAs, dotted green: As(4s) in InAs, solid red: As(4p) in GaAs, dotted red: As(4p) in InAs.

Figure 14. The relative energy differences between $\Gamma \& X$ (olive) and $\Gamma \& L$ (blue) at the CB for unstrained Ga and In series binaries (figure S15).
5. Conclusions

We calculated the strain-induced bandgap variation for various III-V binary compounds focusing on GaAs and GaP for a detailed analysis. We investigated compressive and tensile strain in the range of ±10% around the unstrained structure, which enabled the tuning of the bandgap over a wide range. Furthermore, we showed the presence of direct-to-indirect and indirect-to-direct transitions in the nature of bandgap of these materials based on the analyses of differences between valence and conduction band energies at the $\Gamma$-point ($\Delta E_{\Gamma}$) and the bandgap ($E_g$). Only 4 special k-points were found to be responsible for the direct-indirect transitions: $\Gamma$, L, $\Delta m$, and X. The valence band maximum stayed at the $\Gamma$ point throughout the strain regimes applied. Thus, the position of the conduction band minimum alone in reciprocal space determined the nature of the band gap. By combining the biaxial and uniaxial strain, we proposed a strategy for the realization of direct-indirect transitions in the regions where otherwise no transition could be achieved by single type of strain. With this work, we laid the foundation for further efforts with multinary compound semiconductors under strain.

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Table 4. The calculated equilibrium (unstrained) bandgaps, DIT points, and the DIT transitions compared with the experiments.

| System | Equilibrium bandgap (eV) | Isotropic strain DIT (%) | Transitions |
|--------|--------------------------|--------------------------|-------------|
|        | Calculated               | Experiment               | Calculated  | Experiment |
| Si     | 1.19                     | 1.17                     | —          | —          |
| GaP    | 2.36                     | 2.34                     | —          | —          |
| GaAs   | 1.47                     | 1.52                     | $-1.56$    | $-2.75^b$ |
|        |                          |                          | $\Gamma \rightarrow L$ | $\Gamma \rightarrow X$ |
| GaSb   | 0.64                     | 0.81                     | $-1.00$    | $-1.54^c$ |
|        |                          |                          | $\Gamma \rightarrow L$ | $\Gamma \rightarrow L^c$ |
| InP    | 1.43                     | 1.42                     | $-4.40$    | $-5.16$   |
|        |                          |                          | $\Gamma \rightarrow X$ | $\Gamma \rightarrow X$ |
| InAs   | 0.36                     | 0.41                     | $-7.41$    | $-8.17$   |
|        |                          |                          | $\Gamma \rightarrow X$ | $\Gamma \rightarrow X$ |
| InSb   | 0.03                     | 0.24                     | $-5.18$    | $-4.23$   |
|        |                          |                          | $\Gamma \rightarrow L$ | $\Gamma \rightarrow X$ |

a Experimental bandgaps are at 0 K [38, 129].

b Reference [28].

c Reference [28, 157, 158].

— For Si and GaP IDTs are in the tensile strain region.

No experimental data are available.

Figure 15. Correlation between SMT (isotropic strain) and the energy difference between CB and VB at the $\Gamma$-point ($\Delta E_{\Gamma}$) for Ga and In series binaries.
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